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# User's Manual for Kinetics Model and Ozone Isopleth Plotting Package

**Systems Applications, Inc, San Rafael, CA**

**Prepared for**

**Environmental Sciences Research Lab, Research Triangle Park, NC**

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# User's Manual for Kinetics Model and Ozone Isopleth Plotting Package

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July 1978

# USER'S MANUAL FOR KINETICS MODEL AND OZONE ISOPLETH PLOTTING PACKAGE

by

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# PREFACE

This publication contains information on and the computer programs for the Kinetics Model and Ozone Isopleth Plotting Package (OZIPP). OZIPP can be used to estimate maximum ozone concentrations as a function of initial precursor concentrations, transported ozone/precursors, post-0800 emissions and meteorological conditions which are appropriate for a specific city. From these estimates, the program can generate ozone isopleths which are specific to a city under review. These isopleths can then be applied in the Empirical Kinetic Modeling Approach (EKMA) as described in EPA-450/2-77-021a and EPA-450/2-77-021b. EKMA is useful for (1) estimating NMHC and/or $NO_x$ reductions required to attain the NAAQS for ozone and (2) estimating the change in peak daytime ozone concentrations downwind of cities accompanying a specified change in NMHC and/or $NO_x$.

Although the computer program has been checked thoroughly on Univac and CDC computing systems, incompatibilities on other systems may be found. In case there is a need to update this model, revisions will be distributed in the same manner as this report. Revisions may be obtained as they are issued by completing and mailing the form at the front of the manual.

The computer program described in this manual is available on magnetic tape as EPA-600/8-78-014b and can be acquired in either of two ways:

(1) Government and non-profit agencies may obtain a copy of the program by writing:

Chief, Modeling Support Section (MD-14)
Source Receptor Analysis Branch/MDAD
U.S. Enviornmental Protection Agency
Research Triangle Park, North Carolina 27711

(2) Others wishing a copy of the program may purchase it from the National Technical Information Service, Springfield, Virginia 22161, Telephone (703) 557-4650.

# ABSTRACT

The Kinetics Model and Ozone Isopleth Plotting Package (OZIPP) is a computerized model that simulates ozone formation in urban atmospheres. OZIPP calculates maximum one-hour average ozone concentrations given a set of input assumptions about initial precursor concentrations, light intensity, dilution, diurnal and spatial emission patterns, transported pollutant concentrations, and reactivity of the precursor mix. The results of multiple simulations are used to produce an ozone isopleth diagram tailored to particular cities. Such a diagram relates maximum ozone concentrations to concentrations of non-methane hydrocarbons and oxides of nitrogen, and can be used in the Empirical Kinetic Modeling Approach (EKMA) to calculate emissions reductions necessary to achieve air quality standards for photochemical oxidants. This user's manual describes the technical basis, necessary and optional input data, computer code and the use of OZIPP.

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# 1.0 MODEL OVERVIEW

## 1.1 BACKGROUND AND PURPOSE

The Empirical Kinetic Modeling Approach (EKMA) has been developed as a procedure for relating photochemical oxidants (expressed as ozone) to organic compounds and oxides of nitrogen.[1] The EKMA utilizes a set of ozone isopleths (lines of equal concentration) which depict maximum afternoon concentrations of ozone downwind from a city as a function of the following parameters:

- Morning concentrations of non-methane hydrocarbons (NMHC) and oxides of nitrogen ($NO_x$)
- Emissions of NMHC and $NO_x$ occurring during the day
- Meteorological conditions
- Reactivity of the NMHC mix
- Concentrations of ozone and precursors transported from upwind areas.

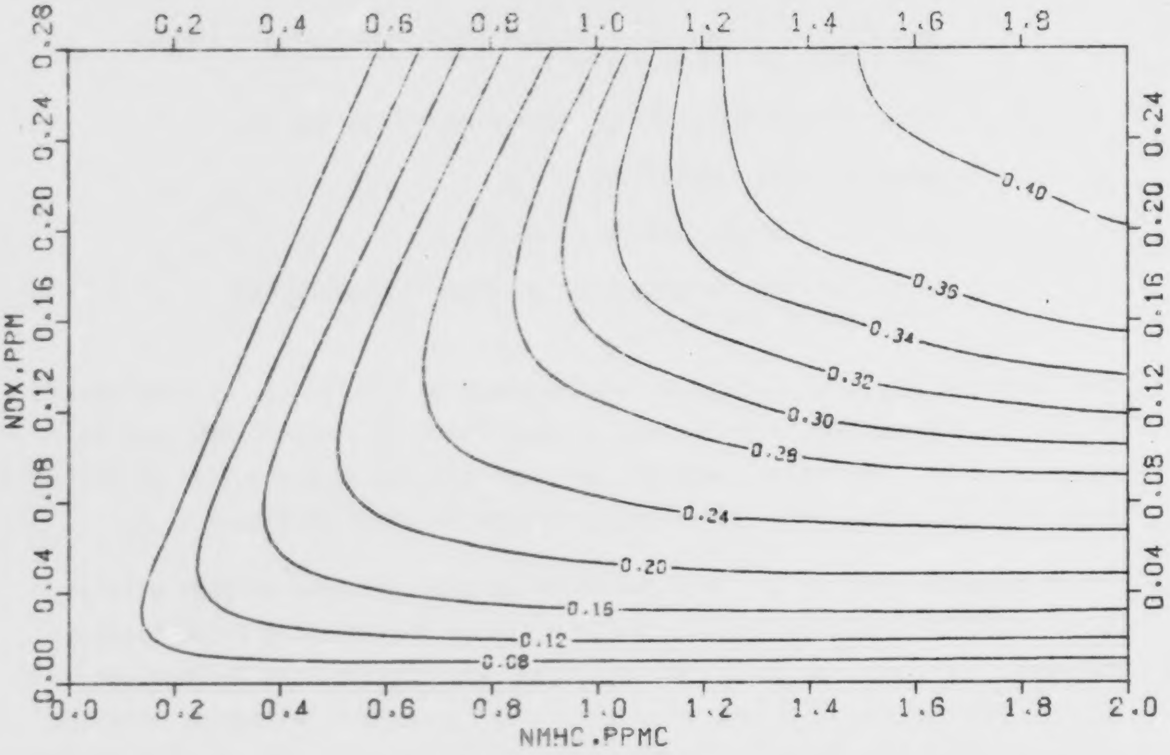
The isopleths are developed by performing computer simulations of atmospheric photochemical reactions with various assumed levels of initial NMHC and $NO_x$ concentrations. The ozone isopleths are then plotted as a function of initial precursor concentrations. (An example diagram is shown in Figure 1-1).

A computer program has been developed to provide users of EKMA with an easy, reliable, efficient and versatile means of constructing ozone isopleth diagrams. This program is called the Ozone Isopleth Plotting Package, or OZIPP. OZIPP allows explicit consideration of transport, different emission patterns, etc. The purpose of this manual is to describe the computer program, the associated input requirements, the information generated and the procedures for executing the program.

## 1.2 SCOPE AND USE

### 1.2.1 Applications

EKMA is a technique for relating changes in the maximum one-hour average ozone concentrations observed within or downwind of an urban area to changes



STANDARD OZONE ISOPLETH CONDITIONS

Figure 1-1. Example Ozone Isopleth Diagram

in the ambient concentrations of NMHC and $NO_x$ in that urban area. It is intended primarily for estimating the emissions controls required in urban areas as part of the State Implementation Plans (SIP) to meet national ambient air quality standards. Thus, EKMA is used to address questions such as:

- What percentage reduction in the ambient concentration of NMHC or $NO_x$, or both, would be needed to attain compliance with the federal air quality standard for photochemical oxidants (ozone)?
- What reduction in the maximum one-hour-average ozone concentration is likely to accompany a given reduction in the ambient concentration of NMHC or $NO_x$?

Procedures for applying the EKMA technique are described in Reference 1. This reference also discusses the derivation of the information which is used in OZIPP.

The primary function of OZIPP is to generate ozone isopleth diagrams that are representative of conditions in a particular city. These types of diagrams, termed city-specific diagrams, are generated by OZIPP using city-specific information on the location and time of year (thereby defining sunlight intensity), local atmospheric dilution rate and local diurnal patterns of NMHC and $NO_x$ emissions. OZIPP can also be used to regenerate the Standard Ozone Isopleth Diagram presented in Reference 1. In this situation, the diagram is based on fixed assumptions regarding sunlight intensity, atmospheric dilution rate and the diurnal pattern of emissions. OZIPP can also be used to simulate ozone formation for a set of city-specific assumptions and specified initial NMHC and $NO_x$ concentrations. When operating in this mode, OZIPP has the capability of displaying the time rate of change of pollutant concentrations, chemical reaction rates, etc.

### 1.2.2 Limitations

EKMA, and therefore OZIPP, is limited in applicability to ozone problems within or immediately downwind of large urban areas. Thus, the OZIPP is not applicable to the following situations:

- The rural ozone problem.
- Situations in which transported ozone and/or precursors are clearly dominant (i.e., a rural area downwind of a city).
- Cases in which the maximum ozone concentration occurs at night or in the early morning.
- Development of control strategies for single or small groups of emissions sources.

The validity of an ozone isopleth diagram generated by OZIPP for a particular city may be limited by the following properties:

- The kinetic mechanism used to describe the transformations of NMHC and $NO_x$.
- The physical assumptions used to formulate the model underlying the isopleths generated by OZIPP.
- The meteorological data and assumptions for specifying the parameters required to apply OZIPP.
- The availability and reliability of current NMHC, $NO_x$ and ozone data.
- The mathematical assumptions needed to solve the differential equations formulated within OZIPP.
- The interpolations necessary to generate isopleths from the results of a number of computer simulations.

Because these factors are part of the basic definitions and concepts that constitute OZIPP and EKMA, they are explained more fully in the following sections.

## 1.3 BASIC DEFINITIONS AND CONCEPTS

### 1.3.1 Basic Definitions

- Kinetic Mechanism -- A kinetic mechanism is a set of chemical reactions and rate constants that is intended to describe some chemical process. From a kinetic mechanism, one can derive coupled, first-order, non-linear differential equations that describe the rates of change of pollutant concentrations with time. These equations can be solved using a computer to simulate the changing pollutant concentrations in a smog chamber or in the atmosphere. The kinetic mechanism used in OZIPP was developed by Dodge[2] and is shown in Appendix A.

- Precursors of Ozone -- Precursors of ozone are the emitted chemical species that react to form ozone. The primary precursors are non-methane hydrocarbons and oxides of nitrogen. In OZIPP, non-methane hydrocarbons are represented by butane and propylene. Methane is not considered a precursor because it reacts very slowly. $NO_x$, as used in this report, signifies the sum of the concentrations of nitric oxide (NO) and nitrogen dioxide ($NO_2$).

- Simulation -- A computer simulation involves the calculation of the concentrations of pollutants included in the kinetic mechanism. Concentrations are calculated at various times beginning at 0800 Local Daylight Time (LDT) and ending at 1800 LDT. The calculations involve the integration of a set of coupled, first-order, non-linear, differential equations that describe the kinetic mechanism and the physical processes underlying the model. User specified assumptions about initial precursor concentrations, emission patterns, dilution, transported pollutants, reactivity and light intensity are incorporated in each simulation.

- Ozone Isopleth Diagram -- An ozone isopleth diagram as generated by OZIPP is illustrated in Figure 1-1. Each curved line in the diagram represents a constant maximum one-hour average ozone concentration. Thus, the NMHC and $NO_x$ coordinates associated with any point on a single, curved line produce the same maximum concentration of ozone. In OZIPP, about 60 simulations are normally performed to produce such a diagram.

- Reactivity -- This is a property of the precursors that governs the rate of ozone production. The kinetic mechanism contained in OZIPP uses a mixture of propylene, which is very reactive, and n-butane, which is only marginally reactive, to represent the reactivity of the NMHC in an urban area.[2] Thus, propylene and n-butane are surrogates for the urban mixture of NMHC, with 100 percent propylene defining the highest possible reactivity and 100 percent n-butane the lowest.

- Default Values -- Certain parameters are necessary for running OZIPP. The default values are the values of these parameters that will be used unless other values are entered in the input data. For example, the default value for the highest initial NMHC concentration used in any simulation is 2.0 ppmC; if no number is entered in the input data for this parameter, OZIPP will use 2.0 ppmC by default. Running OZIPP with all of the default values will generate the standard isopleth diagram described in Reference 1.

- Diagram Point -- Any point on an ozone isopleth diagram generated by OZIPP has three parameters associated with it: an initial NMHC concentration, an initial $NO_x$ concentration and a maximum one-hour average ozone concentration corresponding to the initial NMHC and $NO_x$ concentrations. A set of these three parameters is termed a diagram point. The ozone concentrations at some diagram points are determined from actual computer simulations (i.e., by solving the set of differential equations). The ozone concentrations at other diagram points are interpolated from the simulation diagram points. It is important to note that the NMHC and $NO_x$ diagram points represent only the concentrations of these pollutants resulting from the city's emissions prior to the beginning of a simulation. The precursor concentrations associated with these diagram points do not include pollutant concentrations transported into the urban area, nor the pollutant concentrations resulting from emissions occurring after the beginning of the simulation. Thus, the diagram point precursor concentrations do not necessarily represent the absolute amounts of NMHC and $NO_x$ that generated the ozone in a simulation. However, the ozone concentration associated with each diagram point includes the effects of all these factors.

- Spline Interpolation -- A spline interpolation is the use of a cubic polynomial or a hyperbolic function to interpolate ozone concentrations between diagram points for which ozone concentrations have been calculated by computer simulations. (Interpolation is used to reduce the number of computer simulations necessary to construct an isopleth diagram, and hence to reduce the cost of running OZIPP). Typically, the values of these spline functions and their first and second derivatives are matched at the calculated diagram points, resulting overall in one smooth line that passes through these points. A mechanical analogy of a spline function is a wire constrained to touch certain points. If the wire is pulled taut, it will bend at each point but be straight between points. If the tension is reduced, the wire will provide a smooth curve touching the points. The hyperbolic spline functions used to interpolate between calculated diagram points in OZIPP have an adjustable tension factor analogous to the tension on the wire. However, these interpolations are performed internally by the OZIPP, and normally there is no need for the user to be directly concerned with the spline functions.

### 1.3.2 Concepts

The physical model underlying the OZIPP is similar in concept to a trajectory-type photochemical model. A column of air consisting of initial concentrations of ozone and precursors is transported along an assumed trajectory. As the column moves, it can encounter fresh precursor emissions, which are assumed to be mixed uniformly within the column. The column is assumed to act like a large smog chamber in which the precursors react according to the kinetic mechanism in Appendix A to form ozone and other products. The column extends from the earth's surface to the base of an elevated inversion. The diameter of the column is such that concentrations inside and just outside the column are similar, so that the horizontal exchange of air in and out of the column can be ignored. The volume of the column increases only as the inversion rises. Thus, the pollutants within the column are diluted as they are mixed with the air aloft. If the air aloft is polluted, the inversion rise also introduces ozone and precursors. The OZIPP mathematically simulates these physical and chemical processes.

As discussed in Section 1.2.1, the primary function of OZIPP is to generate an ozone isopleth diagram specific to a particular city. OZIPP operates in two stages. The first stage performs computer simulations to calculate maximum ozone concentrations as a function of initial NMHC and $NO_x$ concentrations. The initial concentrations at which these simulations are performed are carefully selected in such a way as to favor accurate interpolation of the desired ozone isopleths. The first stage, which includes all of the computer simulations using the kinetic mechanism, is by far the most time-consuming part of OZIPP operations. In the second stage, interpolation schemes are used to determine the isopleth lines from the calculated diagram points and to draw the isopleth diagram that is OZIPP's major output.

## 1.4 SYSTEM DESCRIPTION

A schematic diagram of the OZIPP system is presented in Figure 1-2. Note that the off-line plotter is optional. The two major sections of the OZIPP program (i.e., the simulation section and the interpolation and plotting section) are described below.

### 1.4.1 Simulation Section

A schematic diagram of the simulation section is given in Figure 1-3. The input deck activates or suppresses various options in OZIPP and supplies city-specific input data to replace default values. The processor passes the data on sunlight intensity, dilution rate, reactivity of precursors, diurnal pattern of precursor emissions, and data on transported pollutants to the differential equation intergrator for use in the simulations. The information

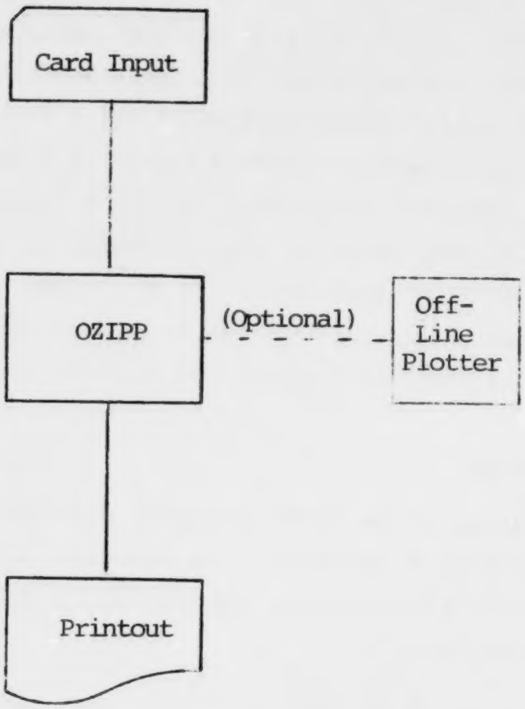

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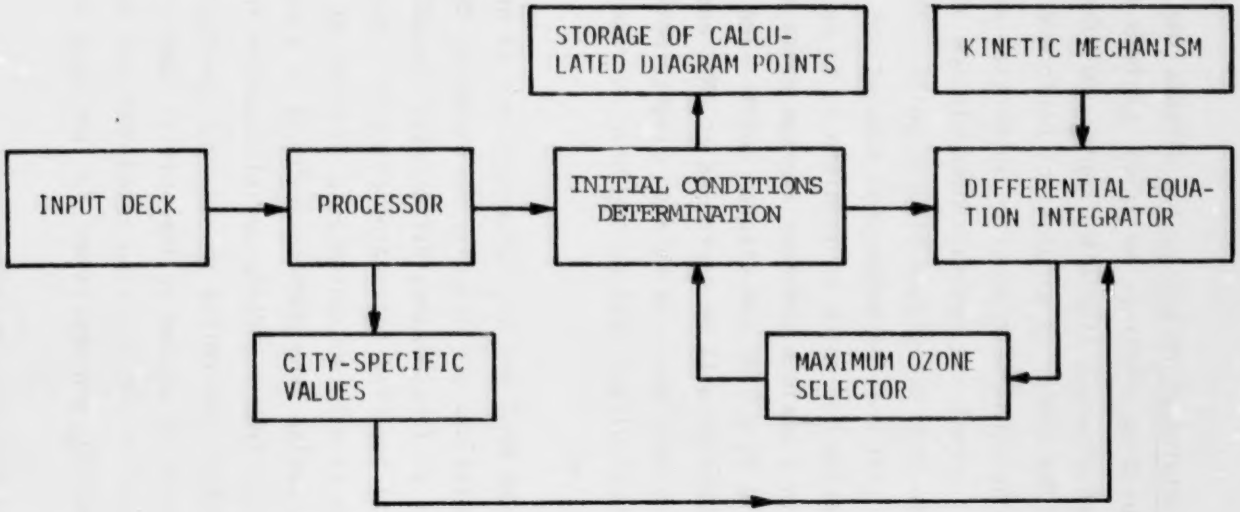
Figure 1-2. Schematic of OZIPP System



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INITIAL CONDITIONS DETERMINATION
STORAGE OF CALCULATED DIAGRAM POINTS
KINETIC MECHANISM
DIFFERENTIAL EQUATION INTEGRATOR
MAXIMUM OZONE SELECTOR

Figure 1-3. Schematic of Simulation Section

on OZIPP options (described in Chapter 3) is passed to the initial conditions determination subsection.

The initial conditions determination subsection directs the performance of the computer simulations used to construct an ozone isopleth diagram. More simulations may produce a more accurate isopleth diagram, but they increase the cost of running OZIPP. (The number of simulations performed can be varied by the user). The initial conditions determination subsection attempts to select simulations which will permit the optimal interpolation accuracy. It includes a feedback scheme, so that calculated diagram points can be used to determine NMHC and $NO_x$ concentrations for subsequent simulations. For example, if the lowest ozone concentration for which an isopleth is to be drawn is 0.08 ppm, a diagram point with a maximum one-hour average ozone concentration of 0.04 ppm is not as valuable as a 0.08 ppm diagram point. The feedback scheme ensures that few simulations will be performed at NMHC and $NO_x$ concentrations similar to those of a previously calculated diagram point, or at concentrations for which the calculated maximum one-hour average ozone concentration is likely to be very low.

After the selection of the NMHC and $NO_x$ concentrations at which simulations are to be performed, the simulations are actually performed by the differential equation integrator. The set of first-order, differential equations is solved numerically. The differential equation integrator calculates the concentrations of 32 chemical species in the kinetic mechanism as a function of time during the simulation period. (The period from 0800 to 1800 LDT is simulated). The ozone concentrations are passed from the differential equation integrator to the maximum ozone selector, which determines the maximum one-hour average ozone concentration. This value is passed to the initial conditions determination subsection, which uses it and its associated NMHC and $NO_x$ concentrations in choosing new NMHC and $NO_x$ concentrations for the next simulation.

### 1.4.2 Interpolation and Plotting Section

After all simulations have been performed, the calculated diagram points are passed to the interpolation and plotting section (represented schematically in Figure 1-4). In the first interpolation stage, spline interpolation is performed between the calculated diagram points to determine specific NMHC and $NO_x$ concentrations corresponding to a specified ozone concentration (i.e., a level for which an isopleth is to be drawn). Unless the user directs otherwise, there are 11 specified ozone levels ranging from 0.08 to 0.40 ppm. The diagram points for the isopleths are then passed to the second interpolation stage, which uses the spline interpolation scheme to determine the final coordinates for the isopleth points. All coordinates are then passed to the plotting software for generation of the final ozone isopleth diagram.

## 1.5 SUMMARY OF INPUT DATA

For generation of the standard ozone isopleth diagram, city-specific values are not necessary. The default values in OZIPP will produce the standard diagram. (The default values are given in Section 3.1). The more city-specific values the user substitutes for default values, the more city-specific the ozone isopleth diagram produced by OZIPP will be. Values of the city-specific parameters that can be input to OZIPP include the following:

- Latitude
- Longitude
- Time Zone
- Date
- Morning and afternoon inversion heights (also called mixing depths)
- Times at which the inversion starts and stops rising
- Concentrations of NMHC, $NO_x$ and ozone in the air above the inversion layer due to transport aloft
- Concentrations of NMHC, $NO_x$ and ozone transported in the surface layer from upwind of the city
- NMHC and $NO_x$ emissions after 0800 LDT
- NMHC reactivity
- Initial ratio of aldehydes to NMHC
- $NO_x$ reactivity (initial fraction of $NO_x$ that is $NO_2$).

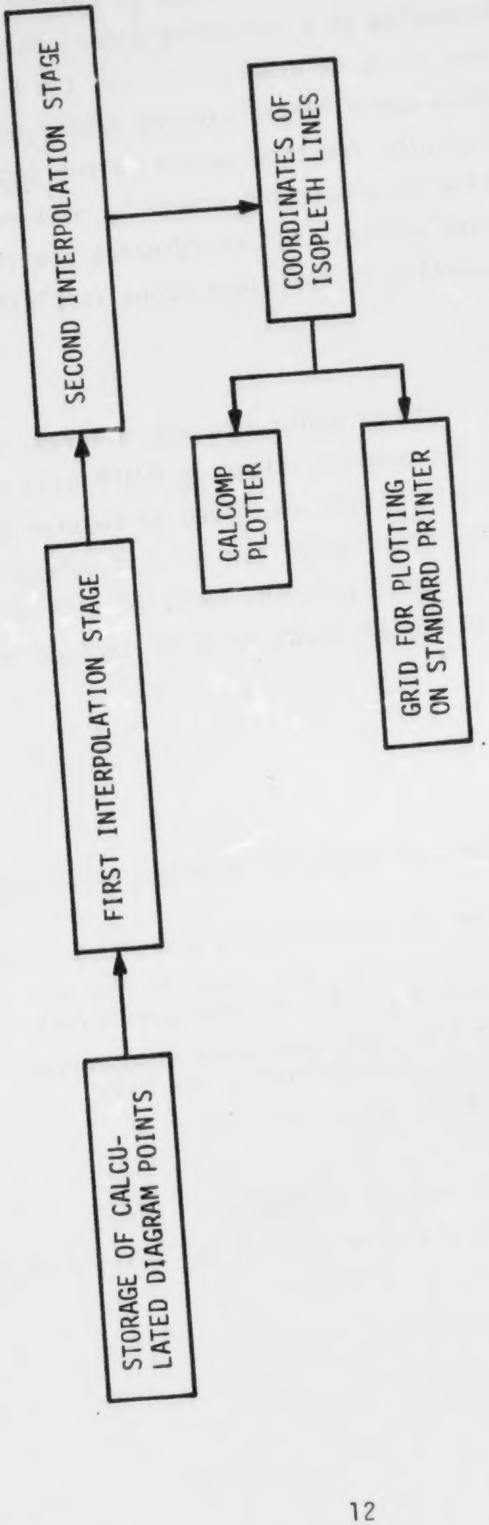
STORAGE OF CALCULATED DIAGRAM POINTS
FIRST INTERPOLATION STAGE
SECOND INTERPOLATION STAGE
COORDINATES OF ISOPLETH LINES
CALCOMP PLOTTER
GRID FOR PLOTTING ON STANDARD PRINTER

Figure 1-4. Schematic of Interpolation and Plotting Section

The sources of values for the parameters in this list and the uses of those parameters in OZIPP are discussed in Chapter 3 and 5.

In addition to city-specific values, OZIPP provides the options of changing several parameters to control its operation. For example, the user can select the number of simulations performed in each OZIPP run, the error tolerance in the differential equation integrator and the form of the output. These input data and options are also described in Chapter 3.

## 1.6 OUTPUT

As previously described, the major function of OZIPP is to produce a city-specific ozone isopleth diagram. The output includes a table summarizing the simulation conditions, a table summarizing the results of each simulation performed, and a line-printer plot of the isopleth diagram. A diagram produced by an off-line plotter (such as CALCOMP) is optional. Under another OZIPP option, a single simulation is performed and the results of that simulation alone are presented. The user also has the option to obtain detailed information for the simulation (e.g., concentrations of all species, rates of reactions, etc.). Examples of OZIPP output are presented in Chapter 5.

## 2.0 TECHNICAL DISCUSSION

OZIPP is designed to simulate ozone formation in urban atmospheres. As discussed in Chapter 1, it consists of two distinct parts. The first part, a kinetics model, mathematically simulates the physical and chemical processes taking place in the atmosphere. The second part, the ozone isopleth plotting package, uses the simulation results to construct an ozone isopleth diagram. This chapter describes the conceptual basis for the kinetics model, the mathematical techniques used in performing a simulation, and the procedures used to generate an ozone isopleth diagram from simulation results.

The descriptions in this chapter are very detailed. Potential users of OZIPP may wish to read the remaining chapters and perhaps run OZIPP once, before reading this chapter.

### 2.1 CONCEPTUAL BASIS FOR THE OZIPP KINETICS MODEL

As previously described, the physical model underlying the kinetics model in OZIPP is similar in concept to a trajectory-type photochemical model. In the kinetics model, a column of air transported along an assumed trajectory is modeled. The column is assumed to extend from the earth's surface to the base of a temperature inversion. The horizontal dimensions of this column are such that the concentration gradients are small. This makes it unnecessary to consider horizontal exchange of air between the column and its surroundings. The air within the column is assumed to be uniformly mixed at all times.

At the beginning of a simulation, the column is assumed to contain some specified initial concentrations of NMHC and $NO_x$ due to prior emissions. The column may also contain NMHC and $NO_x$ that were transported with the column from areas upwind of the city being considered. These pollutants, sometimes called background, are in this report termed pollutants "transported in the surface layer." As the column moves along the assumed trajectory, the height of the column can change because of temporal and spatial variations in mixing height. The height of the column is assumed to change exponentially with time during a user selected period, and to be constant before and after that period.

As the height of the column increases, its volume increases, and air above the inversion layer is mixed in. Pollutants in the inversion layer are described as "transported above the surface layer" or "transported aloft" in this report. Any ozone or ozone precursors from the inversion layer that are mixed into the column as it expands are assumed to be immediately mixed uniformly throughout the column.

The kinetics model in OZIPP can also consider emissions of NMHC and $NO_x$ into the column as it moves along its trajectory. The concentrations of the species within the column are physically decreased by dilution due to the inversion rise, and physically increased by entrainment of pollutants transported aloft and by fresh emissions. All species react chemically according to the kinetic mechanism shown in Appendix A. Certain photolysis rates within that mechanism are functions of the intensity and spectral distribution of sunlight, and they vary diurnally according to time of year and location.

The assumptions and specifications that describe the kinetics model are:

- The air mass of interest is an imaginary air parcel (column) of fixed horizontal area at a constant temperature, within which pollutants are well mixed.
- There is sufficient homogeneity that horizontal diffusion does not affect pollutant concentrations within the column.
- The height of the column varies exponentially with time during a specified period and is constant at other times (an exponential variation is equivalent to a constant percentage dilution per unit time).
- The column contains specified initial concentrations of NMHC and $NO_x$ due to emissions prior to the simulation starting time within the urban area of interest. (These concentrations are shown on the NMHC and $NO_x$ scales of the resulting ozone isopleth diagram). The NMHC is assumed to be 25 percent propylene and 75 percent n-butane, unless changed by the user. Five percent of the initial NMHC concentration is added as aldehydes, unless changed by the user.
- Pollutants transported within the surface layer from outside the urban area of interest (sometimes called background) may be present in the column at the start of each simulation (0800 LDT). The pollutant concentrations due to transport in

the surface layer are normally assumed to be zero, but the user may specify other values for the NMHC, $NO_x$ and ozone concentrations transported within this layer. The NMHC transported within the surface layer is assumed to be 10 percent propylene and 90 percent butane (as carbon). The $NO_x$ transported in the surface layer is assumed to be 100 percent $NO_2$.

- The initial concentrations in the column are thus the sum of the contributions from emissions occurring prior to 0800 LDT plus concentrations transported in the surface layer from upwind locations. Emitted species include propylene, n-butane, NO, $NO_2$, acetaldehyde and formaldehyde. Transported species include propylene, n-butane, $NO_2$ and ozone.

- The changes in pollutant concentrations within the column are calculated, by computer simulation, from 0800 to 1800 LDT. The chemical reactions involving these pollutants are listed in Appendix A.

- Entrainment of pollutants transported aloft is possible during the rise of the inversion layer. OZIPP only permits entrainment of constant concentrations of NMHC, $NO_x$ and ozone. NMHC in pollutants transported aloft is assumed to be 10 percent propylene and 90 percent n-butane (as carbon). No acetaldehyde or formaldehyde is added. $NO_x$ transported aloft is assumed to be 100 percent $NO_2$.

- Pollutants emitted into the column after 0800 LDT can be represented by specifying additions of NMHC and $NO_x$ each hour. The assumptions about the propylene/n-butane and the aldehyde additions are the same as for the initial condition assumptions. The fraction of $NO_x$ that is $NO_2$, however, is 10 percent for post-0800 emissions.

- The rate constants of all chemical reactions in the kinetic mechanism are as shown in Appendix A, except for the photolysis reactions. Photolytic rate constants vary according to the time of day, date and location being simulated. (Default photolysis rate constants are intended to represent the period from 0800 to 1800 PDT on the summer solstice in Los Angeles).

- Zero cloud cover is assumed.

Other assumptions relating to the use of EKMA to predict control requirements or changes in urban ozone concentrations as a result of changes in precursor emissions are discussed elsewhere.[1,3,4]

## 2.2 DESCRIPTION OF A SINGLE SIMULATION

This section describes in considerable detail the mathematical procedures used in OZIPP to calculate the maximum one-hour average ozone concentration that results from given initial concentrations of NMHC and $NO_x$. The procedures are based on the physical and chemical processes described in the last section. Before the beginning of a simulation, data preparation steps are performed. A simulation is conducted by first determining concentrations at 0800 LDT and then numerically integrating the equations that form the basis of the model. The numerical solution yields species concentration as a function of time between 0800 and 1800 LDT. The following discussion describes the data preparation steps, the calculation of initial concentrations, model formulation and the numerical integration technique.

### 2.2.1 Data Preparation Steps

Because all simulations performed by OZIPP in generating an ozone isopleth diagram have identical conditions except for the initial NMHC and $NO_x$ concentrations, a data preparation step is performed before a simulation is commenced. The purpose of this step is to eliminate abrupt changes in photolytic rate constants and post-0800 emission rates. Elimination of these abrupt changes (i.e., discontinuities) is desirable for three reasons:

- The integration scheme requires less computer time (discontinuities require the use of small time steps).
- The results are more accurate numerically (stepping past discontinuities can lead to error).
- The atmosphere does not normally have discontinuities. (The simulation of intermittent cloud cover or sudden changes in emissions is outside the scope of OZIPP).

The photolytic rate constants are evaluated every hour using an algorithm developed by Schere and Demerjian.[5] The algorithm uses input data of latitude, longitude, time zone and date to calculate photolytic constants. A set of third-order polynomial spline functions is then generated so that photolytic constants can be easily calculated from a smooth curve for any time of the day. A set of four coefficients for each of the eight photolytic rate constants in the kinetic mechanism shown in Appendix A is prepared for each hour of the ten-hour simulation period. Thus, at any time during the simulation period, the photolytic rate constants can be calculated from a simple third-order polynomial equation.

If post-0800 emissions are to be considered, it is necessary to specify the emission rate(s) of NMHC and/or $NO_x$ injected into the column each hour after the 0800 simulation start time. These emission rates are expressed as fractions of the initial NMHC and/or $NO_x$ concentrations. They represent the ratio of emissions injected into the column during the specified hour after 0800 to the emissions injected into the air column prior to the beginning of the simulation. A set of cubic spline coefficients is determined each hour so that the instantaneous emission rate(s) can be evaluated for any time during the simulation period. For the first hour, a straight line is used, and for each subsequent hour a simple cubic (or lower order) polynomial is used subject to the following limitations:

- The total, or integrated, emissions for each hour must equal the input value.
- The spline functions at each hour must match in value, slope and curvature unless lower order functions are used.
- At the end of the last hour of post-0800 emissions, the emissions must be zero with zero curvature.
- If cubic splines lead to any minima (points of zero slope) which are less than zero, then a lower order spline function is used for that hour.

### 2.2.2 Determination of Initial Concentrations

Before a simulation can begin, the concentrations of all pollutant species at 0800 LDT must be determined. These initial concentrations are based on assumed initial concentrations of NMHC and $NO_x$ and on the concentrations of pollutants transported in the surface layer. The concentrations of transported pollutants are assumed to be zero unless otherwise specified. If only a single simulation is being performed, the initial concentrations of

NMHC and $NO_x$ must be input to OZIPP. However, if an ozone isopleth diagram is being generated, the initial NMHC and $NO_x$ concentrations are determined internally by OZIPP. This procedure is discussed in Section 2.3.

The concentrations of all but seven species in the kinetic mechanism are initially zero. The concentrations of the other seven species ($NO_2$, NO, $O_3$, propylene, n-butane, formaldehyde and acetaldehyde) are calculated as described below.

1. $NO_2$ is set to the initial $NO_x$ concentration times the $NO_2/NO_x$ fraction (default is 0.25), plus any $NO_2$ transported in the surface layer.

2. NO is set to the initial $NO_x$ concentration times the quantity one minus the $NO_2/NO_x$ fraction. The $NO_x$ transported in the surface layer is assumed to have zero NO.

3. $O_3$ is set to the concentration transported in the surface layer (default is zero).

4. The concentration of propylene is determined from the assumed initial NMHC concentration, the assumed reactivity fraction and the NMHC transported in the surface layer. Mathematically,

$$[C_3H_6]_\circ = \frac{1}{3}\left\{[NMHC]_\circ\,(R_1)+[NMHC]_{ts}(0.1)\right\} \qquad (1)$$

   where

   $[C_3H_6]_\circ$ = initial propylene concentration, ppm

   $[NMHC]_\circ$ = initial NMHC concentration, ppmC

   $R_1$ = fraction of initial NMHC that is assumed to be propylene (Default = 0.25)

   $[NMHC]_{ts}$ = NMHC concentration transported in the surface layer, ppmC

   In equation (1), NMHC transported in the surface layer is assumed to be 10 percent propylene. Multiplication by the fraction $\frac{1}{3}$ converts ppmC to ppm (i.e., there are three carbon atoms per molecule of propylene).

5. The initial concentration of n-butane is determined in a manner similar to the initial propylene fraction.

$$[n\text{-}C_4H_{10}]_o = \frac{1}{4}\left\{[NMHC]_o\,(1-R_1)+[NMHC]_{ts}(0.9)\right\} \qquad (2)$$

where

$[n\text{-}C_4H_{10}]_o$ = initial concentration of n-butane, ppm

$(1-R_1)$ = fraction of initial NMHC concentration assumed to be n-butane (Default = 0.75)

and $[NMHC]_o$ and $[NMHC]_{ts}$ have the same meaning as in Equation (1).

Note that 90 percent of the NMHC transported in the surface layer is assumed to be n-butane. Once again the multiplication by the fraction $\frac{1}{4}$ is necessary to convert from ppmC to ppm.

6. Formaldehyde is initialized according to the initial NMHC concentration and an aldehyde addition factor.

$$[HCHO]_o = [NMHC]_o\,(0.4)\,(R_2) \qquad (3)$$

where

$[HCHO]_o$ = initial formaldehyde concentration, ppm

$[NMHC]_o$ = initial NMHC concentration, ppmC

$R_2$ = fraction of initial NMHC concentration that is to be added as aldehyde (Default = .05)

The fraction of aldehydes assumed to be formaldehyde is fixed at 0.4.

7. Acetaldehyde is initialized similarly to formaldehyde:

$$[CH_3CHO]_o = \frac{1}{2}\;[NMHC]_o\,(0.6)\,(R_2) \qquad (4)$$

where

$[CH_3CHO]_o$ = initial acetaldehyde concentration, ppm

$[NMHC]_o$ = initial NMHC concentration, ppmC

$R_2$ = fraction of initial NMHC concentration to be added as aldehydes

Note that the fraction of aldehyde assumed to be acetaldehyde is fixed at 0.6. Multiplication by $\frac{1}{2}$ converts ppmC to ppm.

### 2.2.3 Mathematical Formulation of Kinetics Model

The kinetics model in OZIPP mathematically simulates physical and chemical processes taking place in the atmosphere. This is accomplished by solving numerically a system of ordinary, non-linear differential equations that describe the effects of these processes on pollutant concentrations. The solution gives the concentration of pollutants as a function of time. The mathematical formulation of the system of differential equations is described in this section.

In OZIPP, there are four processes that are assumed to effect pollutant concentrations:

1) Chemical Reactions
2) Dilution
3) Entrainment of Pollutants Transported Aloft
4) Post-0800 Emissions

Differential equations have been formulated to describe the time rate of change of pollutant concentrations due to each process, and these are presented below. The total time rate of change of each pollutant's concentration is then simply equal to the sum of all these effects. Thus, the system of equations consists of one equation for each species in the kinetic mechanism shown in Appendix A. In OZIPP, however, all equations for species that appear only as products of chemical reactions have been eliminated because of computational considerations. Consequently, the set of equations solved in OZIPP is made up of 32 equations, one for each pollutant appearing as a reactant in any of the 76 reactions in the mechanism.

A. Chemical Reaction Effects

The change in pollutant concentration due to chemical reaction is a function of the rates of the chemical reactions in Appendix A. The rate of each reaction is the product of a rate constant and a concentration term. The rate constants for the non-photolytic reactions are shown in Appendix A. The photolytic rate constants are calculated by the procedures described in Section 2.2.1. The concentration term for unimolecular or psuedo-first-order reactions (such as photolytic reactions) is simply the concentration of the reactant. Bi-molecular reaction rates are calculated similarly, except the concentration term is the product of the two reactant concentrations. For example, the reaction rate (RT) for the first reaction in Appendix A would be expressed as follows:

$$(RT)_1 = k_1 C_{NO_2} \tag{5}$$

where

$(RT)_1$ = rate of reaction (1), ppm $\text{min}^{-1}$

$k_1$ = photolytic rate constant for reaction (1)

$C_{NO_2}$ = concentration of $NO_2$, ppm

The time rate of change of a species due to chemical reaction is simply equal to the sum of all rates for those reactions in which the species is a product minus the sum of the rates for those reactions in which the species is a reactant. Thus,

$$\left(\frac{\Delta C_i}{\Delta t}\right)_R = \Sigma\ (RT)_{PROD} - \Sigma\ (RT)_{REAC} \tag{6}$$

where

$\left(\frac{\Delta C_i}{\Delta t}\right)_R$ = reaction rate contribution to the time rate of change of species i

$\Sigma(RT)_{PROD}$ = the sum of all reaction rates in which species i appears as a product

$\Sigma(RT)_{REAC}$ = the sum of all reaction rates in which species i appears as a reactant

### B. Dilution Effects

The mathematical representation for simple dilution due to inversion rise is a first-order decay process. The rate of change due to this effect can be represented as follows:

$$\left(\frac{\Delta C_i}{\Delta t}\right)_D = -DC_i \qquad (7)$$

where

$\left(\frac{\Delta C_i}{\Delta t}\right)_D$ = dilution effect contribution to the time rate of change of pollutant species i, ppm $\text{min}^{-1}$

$D$ = dilution factor, $\text{min}^{-1}$

$C_i$ = concentration of species i, ppm

The dilution factor is calculated from the following equation:

$$D = \frac{\ln(Z_2/Z_1)}{\Delta t} \qquad (8)$$

where

$D$ = dilution factor, $\text{min}^{-1}$

$Z_2$ = afternoon mixing height

$Z_1$ = morning mixing height

$\Delta t$ = total time during which the inversion rise takes place, minutes

Note that, before and after the inversion rise period, the dilution factor is zero since there are no dilution effects for those periods.

### C. Entrainment Effects

There are only four species subject to being entrained from pollutants transported aloft: propylene, n-butane, ozone and $NO_2$. The mathematical treatment of entrainment assumes that the concentrations aloft do not change with time and extend uniformly to at least the height of afternoon mixed layer. The pollutants entrained are assumed to be instantaneously mixed within the enlarged surface layer. The mathematical expressions for the rates of change for the four pollutants are shown below:

$$\left(\frac{\Delta C_{O_3}}{\Delta t}\right)_{AL} = D(C_{O_3})_{AL} \tag{9}$$

$$\left(\frac{\Delta C_{NO_2}}{\Delta t}\right)_{AL} = D(C_{NO_2})_{AL} \tag{10}$$

$$\left(\frac{\Delta C_{C_3H_6}}{\Delta t}\right)_{AL} = \frac{1}{3}\quad D(0.1)(C_{NMHC})_{AL} \tag{11}$$

$$\left(\frac{\Delta C_{n\text{-}C_4H_{10}}}{\Delta t}\right)_{AL} = \frac{1}{4}\quad D(0.9)(C_{NMHC})_{AL} \tag{12}$$

where

$\left(\frac{\Delta C_{O_3}}{\Delta t}\right)_{AL}$, $\left(\frac{\Delta C_{NO_2}}{\Delta t}\right)_{AL}$, $\left(\frac{\Delta C_{C_3H_6}}{\Delta t}\right)_{AL}$, $\left(\frac{\Delta C_{n\text{-}C_4H_{10}}}{\Delta t}\right)_{AL}$ =

entrainment effect contribution to the time rates of change of ozone, nitrogen dioxide, propylene, and n-butane concentrations, respectively ppm min$^{-1}$

D = dilution factor (i.e., the rate constant for the mixing height rise), min$^{-1}$

$(C_{O_3})_{AL}$ = concentration of ozone trapped aloft, ppm

$(C_{NO_2})_{AL}$ = concentration of $NO_2$ trapped aloft, ppm

$(C_{NMHC})_{AL}$ = concentration of total non-methane hydrocarbon trapped aloft, ppmC

$C_{O_3}$, $C_{NO_2}$, $C_{C_3H_6}$, $C_{n\text{-}C_4H_{10}}$ =

concentrations of ozone, nitrogen dioxide, propylene, and n-butane, respectively, in the mixed layer, ppm

The numerical constants (i.e., 0.1, $\frac{1}{3}$, 0.9, and $\frac{1}{4}$) in Equations 11 and 12 result from the fixed assumptions about the reactivity of the hydrocarbon mix trapped aloft (i.e., 10 percent of the NMHC is assumed propylene) and from the conversion of ppmC to ppm. It should be noted that the effect of the change in mixing height is the sum of the dilution and the entrainment effects.

### E. Post-0800 Emissions Effect

The fourth factor affecting the rate of change of pollutant concentration is post-0800 emissions. The rates of change due to post-0800 emissions are equal to the additional concentrations produced by the emissions. However, recall that the post-0800 emissions are expressed relative to the pre-0800 emissions. For example, for a simulation in which the initial concentration of $NO_x$ due to pre-0800 emissions is 1.0 ppm, and the emissions that occur between 0800 and 0900 are 20% of the pre-0800 emissions, an addition of 0.20 ppm $NO_x$ will occur over the first hour.

Because equivalent emissions into different volumes will produce different concentrations, it is necessary to adjust the relative emissions to reflect the change in the column volumes due to the inversion rise. This is done internally by OZIPP by first calculating the ratio of the 0800 LDT inversion height to the current inversion height. (This is equivalent to the ratio of initial volume to the current volume). Before the inversion rise begins, this ratio is simply one. After the inversion rise has ceased, the ratio is the 0800 mixing height divided by the final mixing height. For the period during which the inversion rises, the ratio ($f_t$) is calculated as follows:

$$f_t = \exp\left[-(D)(\Delta t)\right] \qquad (13)$$

where

$f_t$ = ratio of the 0800 LDT mixing height to the mixing height at time t

$D$ = dilution factor (i.e., the rate constant for the mixing height rise, $\text{min}^{-1}$)

$\Delta t$ = elapsed time between the start of the mixing height rise and the current time, minutes.

The rates of change due to the post-0800 emissions are calculated from the values of the emission rates (calculated using the polynomial spline functions described earlier), the $f_t$ ratio described above, the initial pollutant concentrations and the reactivity assumptions. The equations for the rates of change due to post-0800 emissions for each of the six affected species are shown below:

$$\left(\frac{\Delta C_{NO_2}}{\Delta t}\right)_E = 0.1\ f_t\ (E_{NO_x})_t\ [NO_x]_\circ \qquad (14)$$

$$\left(\frac{\Delta C_{NO}}{\Delta t}\right)_E = 0.9\ f_t\ (E_{NO_x})_t\ [NO_x]_\circ \qquad (15)$$

$$\left(\frac{\Delta C_{C_3H_6}}{\Delta t}\right)_E = \frac{1}{3}\ f_t\ (E_{NMHC})_t\ (R_1)\ [NMHC]_\circ \qquad (16)$$

$$\left(\frac{\Delta C_{n\text{-}C_4H_{10}}}{\Delta t}\right)_E = \frac{1}{4}\ f_t\ (E_{NMHC})_t\ (1-R_1)\ [NMHC]_\circ \qquad (17)$$

$$\left(\frac{\Delta C_{HCHO}}{\Delta t}\right)_E = 0.4\ f_t\ (E_{NMHC})_t\ (R_2)\ [NMHC]_\circ \qquad (18)$$

$$\left(\frac{\Delta C_{CH_3CHO}}{\Delta t}\right)_E = \frac{1}{2}\ (0.6)\ f_t\ (E_{NMHC})_t\ (R_2)\ [NMHC]_\circ \qquad (19)$$

where

$(\quad)_E$ = post-0800 emissions contribution to the rates of change of $NO_2$, NO, propylene, n-butane, formaldehyde and acetaldehyde, ppm $min^{-1}$

$f_t$ = defined above (Eq. 13)

$(E_{NO_x})_t$ = value of post-0800 relative $NO_x$ emission rate, fraction per minute

$(E_{NMHC})_t$ = same as above except for NMHC emissions

$[NO_x]_\circ$ = initial $NO_x$ concentration due to pre-0800 emissions, ppm

$[NMHC]_\circ$ = initial NMHC concentration due to pre-0800 emissions, ppmC

$R_1$ = fraction of initial NMHC (in ppmC) assumed to be propylene

$R_2$ = fraction of initial NMHC (in ppmC) concentration to be added as aldehydes

Note that, in the above formulations, a conversion from ppmC to ppm is performed and that the aldehydes are assumed to be 40 % formaldehyde and 60 % acetaldehyde.

### 2.2.4 Description of Numerical Integration

The kinetics model in OZIPP employs a Gear-type integration scheme to numerically solve the set of differential equations described in the previous section. A detailed description is not given here because the method is not unique to OZIPP, and the procedure has been described elsewhere.[6,7,8] The integration scheme initially uses a time step of $1 \times 10^{-10}$ minutes (i.e., pollutant concentrations are to be calculated $1 \times 10^{-10}$ minutes after the 0800 LDT start time). Subsequent time steps are computed by the Gear-type integration scheme according to the estimated error at each step. However, since the onset and cessation of dilution represent changing conditions, it is necessary for maximal numerical accuracy to begin or end a time step at precisely these points (i.e., the times at which onset and cessation of dilution take place). The pollutant concentrations are calculated at each time step throughout the ten-hour simulation period. (Once the time reaches ten hours, there is no restriction on precisely matching the final time step, since the concentrations can be interpolated back to exactly the tenth hour). A typical simulation in OZIPP takes between 150 and 200 time steps, with about one half of these used in simulating the first minute.

The total rate of change of any species is the sum of the rates of change due to dilution, entrainment, post-0800 emission and chemical reaction described above. At each time step, the concentrations of all species are calculated along with the current rates of change for each species. The Gear method utilizes a Taylor series polynomial for each species to predict the species concentration at the end of the time step. The order of the polynomial is varied internally for optimum efficiency and is based on the values at the beginning of the time step. A corrector scheme then "corrects" the new concentration values, updates the Taylor polynomials and estimates the average error. The corrector is a set of linear equations based on a matrix whose elements are the set of partial derivatives of the rate of change of concentrations of each species with respect to all other species. OZIPP utilizes a linear system solving package for sparse matrices (i.e., those matrices in which most elements are equal to zero). The integration method used in OZIPP has been modified somewhat from the version published in Reference 7. In particular, the error estimation is done relative to the current concentration of a species rather than to its maximum concentration. The method utilizes the error estimate to determine the optimum step size and order, so that the allowable error specified by the user is met with the minimum number of integration steps. For a more detailed discussion of the numerical integration scheme, the user is referred to References 6, 7 and 8.

The final task performed by the differential equations integrator is the calculation of the maximum one-hour average ozone concentration. Ozone concentrations are calculated for precisely every minute of the 10-hour simulation. This calculation is performed by interpolation between the time step solutions to the differential equations. Running one-hour average concentrations are calculated using Simpson's rule. The largest one-hour average concentration is then selected as the maximum.

## 2.3 SELECTION OF SIMULATIONS FOR GENERATION OF ISOPLETH DIAGRAMS

When generating an ozone isopleth diagram, the initial NMHC and $NO_x$ concentrations for each simulation performed by OZIPP are selected in the initial conditions determination subsection (see Figure 1-3). The function of this subsection is to control the selection of initial NMHC and $NO_x$ concentrations in order to obtain as accurate an isopleth diagram as possible from the number of simulations specified. This is accomplished by:

- Performing few simulations for which the maximum one-hour average ozone concentration is below the lowest isopleth to be plotted.
- Minimizing the interpolation error between simulation points when constructing the ozone diagram.

Simulations are first performed at six individual points along the edges of the diagram. Based on these results, simulations are then performed at points along lines of constant NMHC/$NO_x$ ratio (i.e., a radial line emanating from the origin). The user can control the number of radial lines to be considered and the number of points on each radial line. Normally (i.e., under default conditions), simulations are performed at five points along each of 11 radials. Finally, two more simulations are performed for individual points on the edges of the diagram to aid in plotting the lowest valued isopleth. In all, 62 simulations are performed under default conditions.

### 2.3.1 Selection of Individual Points

The first step in the initial conditions determination subsection is to call for four simulations at initial NMHC and $NO_x$ concentrations corresponding to the four corners of the isopleth diagram as shown by points 1 through 4 in Figure 2-1. (Note that the user specifies the maximum NMHC and $NO_x$ concentrations to be used). Next, two simulations (at points 5 and 6) are performed to estimate where the lowest valued ozone isopleth will intersect the diagram edges. The initial conditions for point 5 are determined by using the maximum $NO_x$ value and an NMHC concentration calculated by the following equation:

$$(C_{NMHC})_5 = \frac{(C_{O_3})_{LL} - (C_{O_3})_2}{(C_{O_3})_3 - (C_{O_3})_2} (C_{NMHC})_{MAX} \qquad (20)$$

where

$(C_{NMHC})_5$ = NMHC concentration at point 5

$(C_{O_3})_2$ = $O_3$ concentration at point 2

$(C_{O_3})_3$ = $O_3$ concentration at point 3

$(C_{O_3})_{LL}$ = The lowest ozone value to be plotted as an isopleth

$(C_{NMHC})_{MAX}$ = Maximum NMHC concentration on the diagram

Thus, the coordinates of point 5 are calculated according to the assumption that, at constant initial $NO_x$ concentration, the maximum one-hour average ozone concentration is proportional to the initial NMHC concentration. This

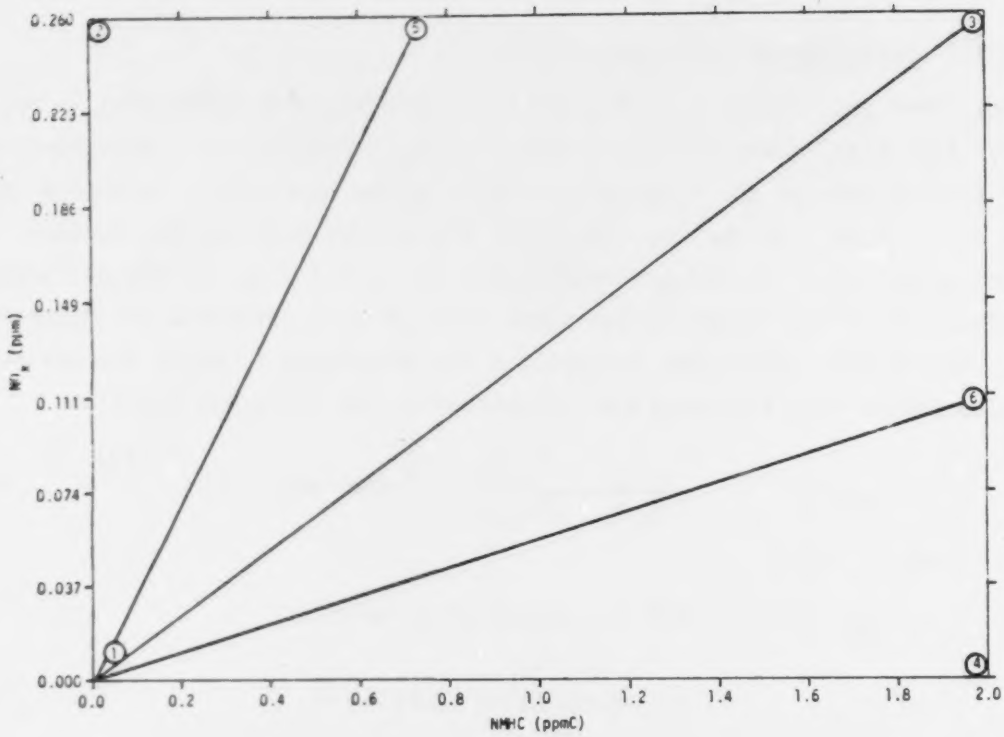

Figure 2-1. Initial Simulation Points

assumption of linearity is generally not true, but the results are used in the next to last simulation in order to calculate a more accurate location. An analogous procedure is performed for the right side of the diagram.

### 2.3.2 Selection of Radials and Points Along Radials

After the simulations are completed for points 1-6, the initial conditions determination subsection directs the simulations at various points along selected radial lines (i.e., lines of constant NMHC to $NO_x$ ratio). The radial lines are used for the following reasons:

- Because most isopleths are roughly L-shaped, simulations at points on radial lines provide the highest density of simulation results near the region of highest curvature.
- Simplified theoretical considerations and empirical evidence show that along any radial line, it is easy to interpolate the maximum one-hour average ozone concentrations as a function of distance from the origin of the isopleth diagram. Typically, these functions are nearly linear at low to intermediate ozone concentrations (e.g., 0.04 to 0.2 ppm ozone) and second order at high concentrations (>0.5 ppm ozone). At the very lowest concentrations, various effects can lead to non-linear behavior, but the functions needed to interpolate along the main part of the radial lines have few inflection points, and therefore the interpolations should have high accuracy.

The first ratio determined corresponds to the diagonal line from the origin of the diagram to the opposite corner (i.e., the point of maximum NMHC and $NO_x$ concentration). Simulations are then performed at various points along that diagonal (the user controls the number of points). The points on the radial are determined by estimating the locations of ozone concentrations along the line. The procedure begins with finding the ozone concentrations that form a geometric progression from the lowest ozone concentration to be plotted (e.g., 0.08 ppm) to the maximum ozone concentration at the terminal point of the radial. A geometric progression gives the minimum relative change in ozone concentration from one point to another. The algorithm is built on the general assumption that the accuracy of the interpolation will be optimized if the relative change in ozone concentration between interpolation points is minimized.

To illustrate the procedure, assume that five simulations are to be performed along the diagonal radial. (Recall that the user can change the actual number of simulation points along the radial). Further, assume that the lowest ozone isopleth to be plotted is 0.08 ppm and that the concentrations of NMHC, $NO_x$ and ozone at the terminal point of the radial are 2.0 ppmC, 0.28 ppm and 0.449 ppm, respectively. In general, the expression for the nth term of a geometric progression is:

$$a_n = a_1 r^{n-1} \qquad (21)$$

where

$a_1$ = the first term

$r$ = the common factor

$n$ = the number of terms

For the example problem, the geometric progression would be:

0.08, 0.12, 0.19, 0.29, 0.449

The common factor (r) was calculated as shown below:

$$r = (0.449/0.08)^{1/4} = 1.54$$

After determining the progression, the next step in the procedure is to estimate the NMHC and $NO_x$ concentrations corresponding to the second highest ozone concentration in the progression (i.e., the first point along the radial below the terminal point). Linear interpolation is used in the following equation to estimate the NMHC concentration associated with this point.

$$(C_{NMHC})_P = (C_{NMHC})_{MAX} \frac{(C_{O_3})_P - (C_{O_3})_1}{(C_{O_3})_{MAX} - (C_{O_3})_1} \qquad (22)$$

where

$(C_{NMHC})_P$ = the NMHC concentration associated with the point

$(C_{O_3})_P$ = the projected ozone concentration associated with the point

$(C_{O_3})_{MAX}$ = the highest ozone concentration in the progression

$(C_{O_3})_1$ = the ozone concentration at point 1

For the example, the NMHC concentration corresponding to the projected 0.29 ppm ozone concentration is 1.30 ppmC. Because the NMHC/$NO_x$ ratio is constant at 7.14 along the line, the associated $NO_x$ concentration is 0.18 ppm. Thus, a simulation is performed with NMHC and $NO_x$ initial conditions of 1.30 ppmC and 0.18 ppm, respectively.

The procedure for determining the locations of subsequent points along the radial is slightly different from the one described above. First, the original geometric progression is updated, using the latest actual simulation result. In the example, the simulation result for the projected 0.29 point was actually 0.34 ppm, so the new progression becomes

.08, .13, 0.21, 0.34

with a new constant factor equal to 1.62. The problem is now one of estimating the location of the 0.21 ozone concentration on the radial. Once again, Equation 22 is used to predict the NMHC concentration associated with the projected 0.21 ozone concentration. However, because two interpolations fairly near each other have been completed (i.e., those giving ozone concentrations of 0.449 and 0.34), a linear extrapolation using these two points is performed to obtain a second estimate. These two estimates are then averaged to obtain the final NMHC value for simulation. This procedure (i.e., new progression, estimation by linear interpolation, estimation by extrapolation, and averaging of the two estimations) is repeated for each point except the last (i.e., the 0.08 point in the example). For this final estimation, a hyperbolic spline interpolation algorithm is employed.

Once all the simulations have been performed for all points on a radial, a new radial is chosen and the procedure repeated. New radials are selected by estimating the location of the terminal points along the top or right edge of the diagram. The scheme for locating the terminal points is essentially identical to the one used in determining the points along the radial. An even distribution of the radial lines is important for obtaining accurate isopleth diagrams. Points too close to each other can introduce erroneous, high-frequency oscillations in the spline interpolations because of errors in the integration scheme. Points too far apart on the isopleth diagram itself leave large areas on the diagram in which no simulations have been performed. The initial conditions subsection contains internal tests on the termination points of the radial lines to avoid these difficulties.

## 2.4 INTERPOLATION AND PLOTTING OF ISOPLETH DIAGRAM

The interpolation and plotting section directs the construction of the ozone isopleth diagram using the results of previous simulations. Interpolation is done with hyperbolic splines rather than with classical polynomial types, because kinetic systems lead to curves resembling exponential functions. A noteworthy feature of the spline functions employed in this algorithm is the tension factor.[9] The highest tension produces straight lines between points, while the lowest value produces roughly cubic fits.

Two stages of interpolation are used to generate the isopleths. In the first stage, the NMHC and $NO_x$ coordinates of the ozone levels to be plotted are determined along each of the radials described in the preceeding section. The second stage draws a smooth curve for each ozone level through the points determined in the first stage. The curves are then plotted using the line printer and, if desired, an off-line plotter such as CALCOMP.

## 3.0 OZIPP OPTIONS AND DATA REQUIREMENTS

As noted earlier, OZIPP contains a complete set of default values which can generate the standard ozone isopleth diagram. The user can obtain other isopleth diagrams by selecting one or more options. This chapter presents the options in OZIPP and their input data requirements. The type of information required for each option is discussed as well as its source, limitations, restrictions and form. Specific information on the format of input data, however, is given in Chapter 4. The use of the options is illustrated with example problems in Chapter 5.

## 3.1 CATEGORIES OF OPTIONS

Data are input to OZIPP by means of option cards with special code words. The options fall into four categories:

- Incorporation of city-specific data.
- Diagram definition (e.g., the number of isopleths to be drawn and the NMHC and $NO_x$ concentration ranges to be condered).
- Methods for reducing computer time.
- Accuracy Tests.

The first two categories are the most important. The last two are available for users who require a means to reduce computing costs or who desire further assurance that the isopleth lines are accurately placed in the diagram.

### 3.1.1 Summary of Code Words and Input Data

The 12 options used to enter data in OZIPP are presented below. Each of these options is identified by a special code word. The input parameters and associated default values for each option are briefly described below. Each of the options and the input data are described in more detail in Section 3.2 and again in Chapter 4.

- ISOPLETH -- This option calls for an isopleth diagram to be constructed according to all specified input parameters. The parameters associated with this option include specification of the maximum NMHC and $NO_x$ concentrations to be considered and selection of the ozone isopleth levels to be drawn. Default values are as follows: maximum NMHC is 2.0 ppmC; maximum $NO_x$ is 0.28 ppm; and 11 ozone levels to be plotted - 0.08, 0.12, 0.16, 0.20, 0.24, 0.28, 0.30, 0.32, 0.34, 0.36 and 0.40 ppm. An additional parameter activates printing solar noon and the time of the center of the maximum one-hour average ozone concentration for each simulation. This information will not be printed under default conditions.

- CALCULATE -- With this option, only one simulation is performed (i.e., only one diagram point calculated) according to the specified input parameters. No isopleth diagram is produced. Initial NMHC and $NO_x$ concentrations must be input with this option. An additional parameter activates the printing of the following: reaction rates, species concentrations, net rates of change in concentrations of all species, and photolytic rate constants for user specified times during the simulation. This information will not be printed under default conditions.

- PLOT -- This option activates the drawing of the isopleth diagram on an offline plotter. Standard CALCOMP routines are used. Input parameters associated with this option control the physical dimensions of the offline plot. Parameters to be specified and their associated default values are as follows: length of abscissa (8.5 inches), length of ordinate (5.95 inches), character and number size (0.10 inches) and label size (0.07 inches). An additional parameter activates the overlaying of a grid of different color on the diagram. Under default conditions, the grid is not drawn.

- TITLE -- This option allows the user to title the program output. Under default conditions, all output is titled "Standard Ozone Isopleth Conditions."

- PLACE -- This option allows determination of the photolysis constants in the kinetic mechanism according to geographical location and time of year. Input parameters associated with this option include the geographic location of the urban area (latitude and longitude), the time zone in which the urban area is located and the time of the simulation. Default values are for a simulation for Los Angeles, California, on June 21, 1975.

- REACTIVITY -- This option allows the user to specify three factors that affect reactivity: the initial fraction of NMHC that is propylene, the initial $NO_2/NO_x$ ratio and the initial fraction of NMHC to be added as aldehydes. Default values for these parameters are 0.25, 0.25 and 0.05, respectively.

- EMISSIONS -- This option permits the consideration of post-0800 emissions. Under default conditions, post-0800 emissions are assumed zero. To override this assumption, the user must specify the fractions of the initial NMHC and/or $NO_x$ concentrations that are to be added each hour to represent the effect of post-0800 emissions.

- TRANSPORT -- This option allows the consideration of transported pollutants. Pollutants can be transported in both the surface layer and aloft. Input parameters include the initial surface layer transported concentrations of NMHC, $NO_x$ and ozone and the concentrations of these pollutants in the air above the base of the inversion layer. All of these concentrations are assumed zero under default conditions.

- DILUTION -- This option allows for the consideration of dilution due to the rise of the inversion layer. Input parameters include the height of the inversion layer in the morning, the final height of the inversion after the rise, the time at which the rise begins, and the time at which the inversion reaches its final height. Under default conditions, the inversion height is assumed to rise from 510 meters at 0800 LDT to 630 meters at 1500 LDT. This represents a 3%/hr dilution rate for the 7 hours between 0800 and 1500.

- ALREADY -- This option permits the use of results from a previous simulation. Input parameters include the initial NMHC concentration, the initial $NO_x$ concentration and the maximum one-hour ozone concentration from each previous simulation. Under default conditions, this option is not exercised.

- ACCURACY -- This option controls the number of simulations, the accuracy of each simultion and the accuracy of the interpolations. Input parameters and their associated default values are as follows: the number of constant $NMHC/NO_x$ radials to be included in the simulations (11), the number of simulations per radial line (5), the error tolerance in the numerical integration scheme (0.01), the tension factor for the first stage of interpolation (1.0) and the tension factor for the hyperbolic spline functions used in plotting isopleths (1.0).

- bbbb (blanks) -- This card terminates the program, and is a required item of input.

### 3.1.2 Structure of Option Cards

To activate an option described in the previous section, a computer card with the appropriate code word must be included with the input deck. Each code must begin in Column 1; however, only the first four characters of each code word are read. Each code word card contains up to six numeric fields, each 10 spaces wide, beginning in Column 11. With some options, one or more subsequent card(s) may be required. These following cards are read either as seven fields of 10 columns each (beginning with Column 1), or as a string of alphanumeric characters. The format for each option card is described in detail in Chapter 4.

## 3.2 DETAILED DESCRIPTION OF OPTIONS

This section describes the options available in OZIPP, the input necessary for each option, and the proper form, card and field for each input value. Chapter 4 presents much the same information from a different point of view, namely, an index of the input data corresponding to each card. The options are described by category below, but note that this order is not the typical order of cards in a deck, CALCULATE and ISOPLETH usually being the next-to-last cards (see Section 5.2).

### 3.2.1 Incorporation of City-Specific Information

Five options are used to input information that is specific to the city under consideration. The input data fix the simulation assumptions about light intensity, dilution, post-0800 emissions, transport and reactivity.

#### A. Place and Date

In all OZIPP runs, the rate constants of the photolysis reactions in the kinetic mechanism are varied in accordance with the diurnal change in sunlight intensity from 0800 to 1800 LDT. This diurnal variation is calculated using a computer code written by Schere and Demerjian[5] which is incorporated in OZIPP. The user can adjust the photolysis rate constants to the area of interest by changing the date or location, or both, from the default values of 21 June 1975 at Los Angeles, California. The option is activated by the code word PLACE. The first three numeric fields of the PLACE card (Columns 11 through 40) contain the latitude (decimal degrees North), longitude (decimal degrees West) and time zone (hours from Greenwich Mean Time). The next three fields are used to specify the year, month and day in Columns 41-50, 51-60 and 61-70, respectively. An additional card may be required to follow the PLACE card. On this card, the name of the city of interest is entered between Columns 1 and 24. This card is necessary only if a non-zero value for the latitude or the longitude is entered on the PLACE card. Therefore, even if the default values of 34.058 and 118.250 are entered, a second card is required with the name of the place. Users interested in the default location need not specify the latitude and longitude.

The correct set of numerical time zones for the continental United States is as follows:

| Numerical time zone | Common name |
|---|---|
| 5.0 | Eastern Daylight Time |
| 6.0 | Central Daylight Time |
| 7.0 | Mountain Daylight Time |
| 8.0 | Pacific Daylight Time |

To produce standard time simulations, even though the output will show daylight time units, a false time zone of one unit (hour) more can be used. Thus, Pacific Standard Time photolysis constants would be generated if a 9.0 was entered instead of the correct 8.0 time zone. The output should then show that solar noon occurs near 1200 hours when the printing of solar noon is activated.

## B. Dilution Rate

The only form of dispersion incorporated in OZIPP is dilution resulting from the rise in the early morning inversion. Under default conditions, the inversion is assumed to rise from 510 meters to 630 meters over a 7 hour period, starting at 0800 LDT. It is assumed that the rise is exponential in nature. This corresponds to an exponential decay in concentration where the decay constant is calculated as follows:

$$D = \frac{\ln (Z_2/Z_1)}{\Delta t}$$

where

$D$ = dilution factor, $\text{min}^{-1}$

$Z_1, Z_2$ = the morning and afternoon mixing heights, respectively (any consistent units)

$\Delta t$ = the length of time over which the change in mixing height occurs (minutes)

For the default values, the value of the dilution factor is $5.03 \times 10^{-4}\ \text{min}^{-1}$. This corresponds to a dilution rate of about 3 percent per hour.

City-specific values for determining the dilution rate are entered using the word DILUTE. The values of the morning mixing height, afternoon mixing height, inversion rise starting time and inversion rise stopping time are entered in the first four numeric fields of the DILUTE card (i.e., Columns 11-20, 21-30, 31-40 and 41-50, respectively). The starting and stopping time should be in 24-hour time format, LDT. For both default and specific conditions, dilution is assumed not to occur outside the starting and stopping times.

### C. Post-0800 Emissions

OZIPP has the capability of treating emissions of NMHC and $NO_x$ that occur after 0800 LDT. (Recall that under default conditions, these emissions are assumed to be insignificant and, thus, zero). The post-0800 emissions are meant to reflect only those emissions injected into the imaginary column of air after the beginning of the simulation. They are expressed relative to the emissions injected into the column of air prior to the 0800 LDT simulation starting time. The pre-0800 emissions are represented by the initial NMHC and $NO_x$ concentrations. The post-0800 emissions are represented by hourly additions to these concentrations. Thus, the post-0800 emission input values are actually the fractions of initial NMHC and $NO_x$ concentrations to be added each hour after the simulation starts. For example, if 20% of the pre-0800 $NO_x$ emissions occur during the first hour, 20% of the initial $NO_x$ concentration (excluding transported pollutant concentrations) would be added to the column concentration between 0800 and 0900 LDT.

The reactivity of organic emissions is assumed to be the same as for the initial concentrations [i.e., the same propylene-butane split (ordinarily 75% - 25%) and the same aldehyde to NMHC ratio (ordinarily .05) are used for post-0800 emissions as for pre-0800 emissions]. However, the post-0800 $NO_x$ emissions are assumed to be 90 % NO and only 10 % $NO_2$. This cannot be altered using the OZIPP options.

The fractions of initial NMHC and $NO_x$ to be added each hour are modified within OZIPP to account for the volume change associated with dilution. For example, assuming default dilution conditions, an emissions fraction of 1.0 in the eighth hour of the simulation would be multiplied actually by 510/630 (or 0.81) to account for the larger volume in the air column, because the inversion rose to 630 meters from the original 510 meters. Additional modifications to the input data are performed by OZIPP to smooth out abrupt changes in the emissions.

In developing the input data, three pieces of information are required. The number of hours during which the post-0800 emissions continue must be specified. Then, for each of these hours, the fractions of both NMHC and $NO_x$ initial concentrations to be added must be specified. If the fractions for both pollutants are essentially the same, then only one set of fractions need be input. This single set will be applicable to both pollutants. Reference 1 includes guidelines for estimating post-0800 emissions. These guidelines are also briefly discussed in Section 5.2.

If post-0800 emissions are to be included, a card with the code word EMISSIONS should be used. The second numeric field (Columns 11-20) must contain the number of hours for which post-0800 emissions are to be specified (the maximum is 10). If only one set of emission fractions will be input, and that set will apply to both NMHC and $NO_x$ emissions, the number of hours should be coded as a positive number. Then the emission fractions should be coded in the next five numeric fields and, if necessary, coded on an additional card starting in the first 10 column field (i.e., Columns 1-10). For example, if 10 hours of emissions were to be input, the EMISSIONS cards would contain the first five fractions in fields 3 through 7, i.e., Columns 21-30, 31-40, 41-50, 51-60 and 61-70 (recall that only the first seven fields are normally used in OZIPP option cards). The next card would contain the fraction for the sixth through the tenth hours, with the fractions for the sixth hour coded in Columns 1-10, the fractions for the seventh hour coded in Columns 11-20, etc.

If different fractions for NMHC and $NO_x$ are to be used, the number of hours for which post-0800 emissions are to be input should be coded as a negative number in the second field of the EMISSIONS card. The NMHC fractions are coded exactly as described above. The first $NO_x$ fraction is then entered in the first field (Columns 1-10) on a card immediately following the NMHC fractions. The remaining $NO_x$ fractions are coded in the following fields or this card and additional cards, if necessary.

If it is desired to input emissions for only one pollutant, it is not necessary to code zeros for the other pollutant's emission fractions. Any negative number coded for the first hour's fraction will indicate to OZIPP that no fractions are to be input for that pollutant. Thus, if no NMHC emissions are to be added, a negative number coded for the first NMHC fraction will cause OZIPP to skip immediately to the next card and to process $NO_x$ fractions. Likewise, a negative number for the first $NO_x$ field will cause OZIPP to skip the next card and to begin processing the next option.

### D. Transported Concentrations

OZIPP's default conditions do not include any pollutants transported from upwind areas. However, the TRANSPORT option is available to include the effects of ozone and precursors transported from areas upwind of the city of interest. Two types of transport can be included. The first type results from the transport of pollutants into the urban area within the surface layer. The second type results from pollutants being transported within air masses trapped above the mixing height at night. As the mixing height rises during the day, the transported pollutants trapped aloft are entrained into the mixing layer. For both types of transport, the following assumptions about precursor reactivity are made:

1) 10% of the transported NMHC concentration is propylene, 90% n-butane
2) No aldehydes are transported into the area
3) All transported $NO_x$ is $NO_2$.

These assumptions cannot be changed by the user.

Concentrations of $O_3$, NMHC and $NO_x$ transported in the surface layer are entered in the first, third and fifth numeric fields of the TRANSPORT card (Columns 11-20, 31-40 and 51-60, respectively). The appropriate units for $O_3$ and $NO_x$ are ppm, and for NMHC the units are ppmC. Subsequent simulations will have these concentrations added to the initial concentrations. Thus, the actual initial NMHC and $NO_x$ concentrations simulated will be the sum of the diagram point values and the values transported in the surface layer.

The treatment of pollutants being entrained from aloft is also activated with the same TRANSPORT card. The concentrations of $O_3$ (ppm), NMHC (ppmC) and $NO_x$ (ppm) in the air aloft are entered in the second, fourth and sixth numeric fields of the card (Columns 21-30, 41-50 and 61-70, respectively).

### E. Reactivity Changes

The reactivity of the ozone precursors can be modified by changing any of three factors: the hydrocarbon mix* (i.e., the fraction of NMHC assumed to be propylene), the fraction of the initial $NO_x$ concentration that is $NO_2$, and the fraction of the initial NMHC concentration that is added as aldehyde. Any one or all of these factors can be changed by using a card with the code word REACTIVITY before the ISOPLETH or CALCULATE cards. A number entered in the first numeric field (Columns 11-20) of REACTIVITY will replace the default value of 0.25 for the fraction of initial carbon atoms in the form of propylene. A number in the next field (Columns 21-30) replaces the default initial

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* Although this capability exists, at the present time it is uncertain how to characterize reactivity of mixtures differing greatly from automobile exhaust in terms of propylene to NMHC ratios.

$NO_2/NO_x$ ratio of 0.25, and a number in the third field (Columns 31-40) replaces the default value of 0.05 for the fraction of initial carbon atoms added as aldehydes. (The initial aldehyde concentration is assumed to be 40 % formaldehyde and 60 % acetaldehyde as ppmC).

### 3.2.2 Diagram Definition Options

The possible modifications to the form of the isopleth diagram constructed by OZIPP are described below.

#### A. NMHC and $NO_x$ Concentration Ranges

In all OZIPP isopleth diagrams, the origin represents 0.0 ppmC NMHC and 0.0 ppm $NO_x$. The maximum NMHC and $NO_x$ concentrations represented on the abscissa and the ordinate can be changed from their respective default values of 2.0 ppmC NMHC and 0.28 ppm $NO_x$ by putting the desired maxima in the first two numeric fields of the ISOPLETH card. The desired maximum NMHC concentration (in units of ppmC) should be punched in the field of Columns 11 through 20. The desired maximum $NO_x$ concentration (in units of ppm) should be punched in the field of Columns 21 through 30.

Any number may be used for the desired maximum NMHC or $NO_x$ concentrations, but because the scales on the abscissa and the ordinate are divided into ten and seven divisions, respectively, only certain values of the maxima will produce even markers. Thus, to produce an easy-to-use diagram, the $NO_x$ maxima should be evenly divisable by seven (e.g., .07 ppm, .14 ppm, .21 ppm, .28 ppm, etc). Similar considerations should be given to selecting a NMHC maximum.

#### B. Number and Spacing of Isopleths

The desired number of isopleths in the diagram should be inserted (followed by a decimal point) in the field of Columns 31 through 40 of the ISOPLETH card. Up to 20 isopleths can be drawn (the default value is 11). OZIPP then reads the proper number of fields from the succeeding card or cards to find the ozone concentrations (in units of ppm) for which isopleths are to be drawn. For example, inserting 10.0 in Columns 31-34 of ISOPLETH causes OZIPP to read the seven 10-space numeric fields on the next card and three on the succeeding card. (As noted earlier, OZIPP does not read past Column 70 on any card except the program title card).

## C. Title

The title can be changed by inserting a card with the code word TITLE followed by a card with the desired title. Everything in Columns 1 through 72 of this title card will be printed on the output and isopleth diagrams in place of the default title, "Standard Ozone Isopleth Conditions." As with all options, these cards must precede the ISOPLETH or CALCULATE cards.

## D. CALCOMP Plotting

Any plotting package that can be called using standard CALCOMP subroutines can be used. Calls to these routines are activated by a card with the code word PLOT. This card must precede the ISOPLETH card. The actual CALCOMP routines called are PLOTS, PLOT, NUMBER, SYMBOL and NEWPEN (if necessary). The use of the CALCOMP routines is discussed in Section 4.3.2.

The user also has the option to specify the actual size of the plot by defining the lengths (in inches) of the sides of the diagram. Columns 31-40 are used for the abscissa of the diagram. Columns 41-50 are used for the ordinate of the diagram. The size of title characters and axes numbers and the size of the isopleth labels can also be set by the user in Columns 51-60 and 61-70, respectively. The default values were given in Section 3.1.1. If the user wishes to reset any of these values, it is recommended that all values change proportionally.

Another option on the CALCOMP plots is the overlay of gridded lines on the isopleth diagram. This is done by declaring any non-zero positive value in Columns 21-30. If this option is exercised, a grid of different color will be overlayed onto the diagram. If the user does not have access to the choice of different pen colors, it is not recommended to use this option. For users with access to a matrix plotter (such as the VERSATEC plotter), and the choice of lines consists of thickness and patterns (i.e., dot-dash, on solid patterns) then the user may enter a negative non-zero value in Columns 21-30. The absolute value of the number entered represents the user's choice of pattern and thickness. This number varies with different computer systems.

### 3.2.3 Methods for Reducing Computer Time

Most of the computing time of an OZIPP run is expended in performing simulations. OZIPP performs simulations at diagram points located along straight lines radiating from the origin of the isopleth diagram. In other words, OZIPP performs several simulations on each of a number of lines of constant NMHC/$NO_x$ ratio. The number of radial lines (i.e., lines of constant NMHC/$NO_x$ ratio) and the number of simulations per line can be varied by the user. (OZIPP also performs simulations at the corners of the isopleth diagram and elsewhere that cannot be controlled by the user).

A means of reducing computer costs is often necessary, so several options are available in OZIPP to allow such savings. For example, fewer radial lines and fewer simulations per line in OZIPP can produce an isopleth diagram at lower cost. However, the isopleths will have been interpolated from fewer points. For control strategy usage, the default values of eleven radial lines and five simulations per line are recommended. Much computer time can be wasted by a poor choice of maximum initial NMHC and $NO_x$ concentrations on the abscissa and the ordinate of the isopleth diagram. When city-specific options are activated, some of the isopleth lines desired by the user may be off the diagram specified or may be cramped into a small part of the diagram. In addition, CALCOMP plotting may require extra time or added expense. In such cases, trial OZIPP runs without the CALCOMP option can be made with the number of simulations reduced. Then, the maximum NMHC and $NO_x$ values that produce the best display of the ozone isopleth lines can be determined. This is discussed further in Section 5.2.

#### A. Radial Line Control

The number of radial lines used in construction of the isopleth diagram can be controlled by specifying the desired number of lines (any odd number from 1 to 19) in the first numeric field (Columns 11-20) of the ACCURACY card. Leaving this field blank produces the default value of 11.

### B. Number of Simulations Per Radial

This number is controlled using the second field of the ACCURACY card (Columns 21-30). The possible values are 1 through 8 and the default value is 5. Thus, the isopleth diagram requiring the least computer time would result from a 1.0 in both of the first two numeric fields on the ACCURACY card. Essentially, only the diagram points at the corners of the diagram would be simulated. These results would be useful in estimating the NMHC and $NO_x$ concentrations that define the limits of an isopleth diagram.

### C. The Use of Previous Simulation Results

The results from previous simulations can be utilized with the card coded with ALREADY. In order to incorporate results from a previous run, the following conditions must be identical in both runs: the NMHC and $NO_x$ scales, the city-specific options, number of radial lines and the number of simulations per line. Such a situation could occur when:

- An initial run may have terminated because of time restriction
- The user may wish to repeat the run with PLOT option in order to obtain a CALCOMP generated plot
- The user may wish to alter the tension factors used in the interpolation schemes.

To input the results of previous runs, the number of completed simulations is entered in the first numeric field (Columns 11-20) of the ALREADY card. The results of those simulations must be entered on the following cards in the same order in which they are calculated. Each card contains the results of one simulation. Field 1 (Columns 1-10) contains the initial NMHC concentration, Field 2 (Columns 11-20) initial $NO_x$ concentration and Field 3 (Columns 21-30) the resulting maximum one-hour average $O_3$ concentration.

## D. First Ozone Peak

A considerable amount of computer time is wasted when the maximum one-hour average $O_3$ concentration in a simulation occurs early but the simulation is continued for the full ten hours. The default condition in OZIPP forces this continuation because two ozone peaks often occur in simulations, and the second may be the larger. Nevertheless, a sizeable reduction in computer costs is possible for simulations with single ozone peaks if the simulations are stopped after their peaks are reached. This can be done in OZIPP by placing any number in the sixth numeric field (Columns 61-70) of the ACCURACY card. However, the reasons for two ozone peaks are not well understood, so the full 10 hours must be used to generate isopleth diagrams intended for control strategy usage.

## E. Multiple Isopleths or Calculations

Any number of isopleth diagrams or individual calculations can be performed in one run of OZIPP. The user merely needs to insert the desired number of ISOPLETH and CALCULATE cards. One set of simulations and an associated ozone isopleth diagram will be produced for each ISOPLETH card. Likewise, a single simulation will be performed for each occurrence of the CALCULATE card. Except for options that cannot be deactivated, all options activated will remain in effect until respecified. Likewise, all input data will be fixed until redefined. Thus, if the default value for a parameter is desired in place of a value specified earlier, the default value must be respecified.

Once activated, the following two options cannot be turned off: PLOT, and the first ozone peak option of ACCURACY. If the ALREADY option has been activated, it also will remain activated until turned off (i.e., previous simulation results will be used with all subsequent ISOPLETH options). To deactivate the ALREADY option, another ALREADY card must be entered with a zero or blanks in the first numeric field (Columns 11-20).

To illustrate the procedure for obtaining multiple diagrams, assume that it is desired to produce two ozone isopleth diagrams. One diagram is to reflect default dilution conditions, and the second diagram different assumptions about dilution. The option cards might then be ordered as follows:

1) a set of cards specifying all options and input values other than dilution (thereby invoking default dilution conditions)

2) an ISOPLETH card causing an ozone isopleth diagram with default dilution condition to be produced

3) a DILUTION card specifying the new dilution condition

4) an ISOPLETH card causing an ozone isopleth diagram with the new dilution conditions to be produced.

Note that two sets of simulations are performed, and that the same results could be accomplished with two separate runs.

### 3.2.4 Accuracy Tests of the Isopleth Diagram

Options have been incorporated into OZIPP to allow users to test the accuracy of the diagram. In this manual, the term "accuracy" is always used in reference to the numerical solution of an implied initial value problem in ordinary differential equations. Thus, accuracy does not refer to the degree of correspondence between an isopleth diagram and atmospheric data.

Although the extensive experience gained in the development of OZIPP suggests that the default radial lines, number of simulations per line, tension factor, and so on, will generate sufficiently accurate isopleth diagrams, this experience does not guarantee sufficient accuracy. The recommenced procedures to check many of the factors that affect accuracy are similar. They merely answer the following question: Do somewhat higher or somewhat lower values of the factor significantly affect the resulting isopleth diagram? OZIPP has been designed to respond properly to these factors. For instance, an increase in simulation density (more radial lines or more simulations per line) should produce a more accurate isopleth diagram. The procedures in OZIPP to check accuracy and to generate additional information are discussed below.

### A. The Density of Simulations

As described above, the number of radial lines and the number of simulations per line can be decreased to reduce computer time using the ACCURACY card. These numbers can also be increased to check accuracy. The first numeric field (Columns 11-20) on ACCURACY specifies the number of radial lines, and the second field (Columns 21-30) the number of simulations per radial line. The limits of acceptable input are odd numbers from 1 to 19 for the former and any number from 1 to 8 for the latter.

The accuracy of the points at which isopleths touch the edges of the diagram can be checked (with minimal computer cost) by specifying 19 lines and 1 calculation per line. The accuracy of the isopleth lines along the diagonal of the isopleth diagrams can be checked by specifying 1 radial line and 8 simulations per line. The spacing and values along any one radial line can be checked by adjusting the diagram to make that line the diagonal (using the ISOPLETH card) and using the ACCURACY card with 1 radial line and 8 calculations on that line. (The ISOPLETH card must follow the ACCURACY card).

### B. Calculation at Specified Points

Individual simulations can be performed at specified initial NMHC and $NO_x$ concentrations using the CALCULATE card. This option might be required to check an interpolated point or to gain more information about a simulation actually performed on a previous isopleth diagram. The first two numeric fields on the CALCULATE card (Columns 11-20 and 21-30) must specify the desired initial NMHC and $NO_x$ concentrations. The initial conditions and hourly ozone concentrations will be printed to show the change of ozone in the simulation with time. Any number entered in the third numeric field (Columns 31-40) will activate an information option that will print:

- The rate constants used in the kinetic mecahnism.
- The concentrations of all species in the kinetic mechanism.
- The net rate of change of all species.
- The reaction rates for each reaction.
- The photolysis constants for all photolysis reactions.

If the information option is activated, the user may specify the simulation time (in minutes) for which concentrations of all species, current reaction rates, etc., will be printed. The number of minutes after the simulation starting time at which the initial printing is made (Default value = 60 minutes after start) is entered in Columns 41-50. The integral time step for which subsequent printings are made (Default value = 60 minutes) is entered in Columns 51-60. Under default values, hourly concentrations of species, net rates of change, etc., are printed.

After the simulation has ended, a concentration versus time profile is printed for ozone. An example of output from this option is given in Chapter 5.

## C. Accuracy of Simulations

The numerical integration scheme employed in OZIPP estimates the error at every step of the integration. The size of the time step taken by the computer is adjusted to keep the estimated error in the range specified. The error is conveniently controlled by a single parameter with a default value of 0.01. Smaller values of this parameter increase both the accuracy and computer time. Larger values do the opposite. By entering numbers smaller than 0.01 in the third numeric field of the ACCURACY card (Columns 31-40), one can estimate the accuracy of the simulations. For example, if several CALCULATE and ACCURACY cards are used, several simulations can be performed with the same initial NMHC and $NO_x$ concentrations but with different time steps in the numerical integration. This procedure can be used to demonstrate how the simulation results vary with increased error tolerance. Table 3-1 shows the results of such a test using the default conditions.

## D. Spline Interpolation Accuracy

There are two parameters that can be used to control the spline interpolation schemes. Normally, the default values are perfectly adequate. The parameters should only have to be modified under rare circumstances. Consequently, the following discussion is included primarily for thoroughness.

TABLE 3-1. MAXIMUM OZONE CONCENTRATIONS IN SIMULATIONS AT VARIOUS ERROR TOLERANCES IN THE NUMERICAL INTEGRATION

| Maximum Ozone Concentration (ppm) | Error Tolerance |
|---|---|
| 0.28624 | 0.00001 |
| 0.28617 | 0.0001 |
| 0.28581 | 0.001 |
| 0.28602 | 0.01 (default) |
| 0.28158 | 0.1 |
| 0.28158 | 0.2 |
| 0.27957 | 0.5 |

NOTE: In all simulations, the initial NMHC concentration was 1.0 ppmC, the initial $NO_x$ concentration was 0.13 ppm and the default values were used for all other variables.

Unfortunately, the spline functions used to interpolate between simulation results do not have a parameter as relevant to accuracy as does the numerical integration scheme used for the simulations. The spline functions can be controlled to a limited extent by a simple factor analogous to tension. The lowest values (e.g., 0.001) cause the hyperbolic spline function to resemble cubic splines, and high values (e.g., 50.0) result in virtually straight lines between points or linear interpolation. Since two stages of interpolation are used in OZIPP, there are two parameters available to control tension. Default values for both are 1.0, and control is obtainable by entering the desired number in the fourth and/or fifth numeric fields of the ACCURACY card (Columns 41-50 and 51-60). The first factor controls the first stage, namely interpolation between diagram points along the top edge of the isopleth diagram, along the right edge and along each radial line. This interpolation stage estimates the coordinates of ozone concentrations for which isopleths are to be constructed. The second stage interpolates between diagram points calculated in the first stage to generate the coordinates of the isopleths themselves. Thus, a value of 50.0 in the fourth numeric field of the ACCURACY card would cause nearly linear interpolation to be used to locate the diagram points on the radial lines and edges that correspond to the ozone concentrations at which isopleths are to be drawn. A value of 50.0 in the fifth field would result in nearly straight lines between diagram points calculated in the first stage.

To a limited extent, the tension factor for the first stage of interpolation controls the selection of initial NMHC and $NO_x$ concentrations for some simulations because the same interpolation scheme is used in selecting the initial concentrations for the simulations. Therefore, using the results of a set of simulations (via the ALREADY option) with different first stage tension factors may produce slightly different isopleth diagrams.

### 3.3 LIMITATIONS ON ISOPLETH SHAPES

In general, most of the parameters used in OZIPP have a limited range of acceptable values. These have been described in this chapter and the next.

In addition to these limits, there are certain types of isopleths that cannot be plotted by OZIPP. But the designers of OZIPP are not aware of any conditions that would result in isopleths of these types. Among the types of isopleths OZIPP cannot plot are:

- Lines that touch the lower edge.*
- Lines that are closed or that loop in any way.
- Lines that touch the left edge in two places.
- Two or more separate lines at the same $O_3$ concentration (only the line closest to the left edge will be plotted).

---

* As shown in Figure 1, the lower edge of an OZIPP ozone isopleth diagram is at 0.0 initial $NO_x$. The left edge is 0.0 initial NMHC, the top edge the maximum initial $NO_x$ and the right edge the maximum initial NMHC concentration.

## 4.0 USER'S GUIDE

This chapter describes the format of the input data, types of error and warning messages that can occur, and some special problems to consider in installing the program on any one facility. In addition, example job control language is presented for illustration.

### 4.1 FORMAT OF INPUT DATA

The twelve options in OZIPP, which were discussed in Chapter 3, are listed in Table 4-1. For each option, the locations of the different parameters on the appropriate cards are shown. The order of the OZIPP options in the input deck is not important except for the ISOPLETH and CALCULATE options. Any options to be activated for simulations must precede these two options. Consequently, the order shown in Table 4-1 is recommended. This ordering has the TITLE option listed first, followed by the options used to input city-specific information (PLACE, DILUTION, EMISSIONS, REACTIVITY and TRANSPORT). The next group of options affect some of the operational aspects of OZIPP (ACCURACY, ALREADY and PLOT). The two options that actually initiate simulations follow (CALCULATE, and ISOPLETH). The last card of any input set must be a blank card.

**As shown in Table 4-1, all 4-letter code words (e.g., TITL, PLAC, etc.) which activate an option must begin in Column 1. Each card with such a code word has up to six numeric fields, each ten spaces wide, beginning in Column 11. An entry can be made anywhere in a field, but a decimal point must always be used, even with integral values. Some options have additional data cards associated with them. These cards must follow** the option card in the order specified in Table 4-1. For example, the card containing the title must immediately follow the card with the code word TITL. Data cards that do not begin with code words contain 7 ten-column fields beginning in Column 1. Like the numeric fields on cards with code words, entries may be made anywhere in the field provided a decimal is used.

As previously described, most parameters have default values associated with them. These are indicated by DF in Table 4-1. If no entry is made in a numeric field, the default value will be assumed. For example, if the only entry made on the PLACE card is in the first numeric field, the default value of 118.25 will be assumed for the second numeric field, 8.0 for the third, etc.

## TABLE 4-1.
## INPUT FORMAT FOR OZIPP OPTIONS

| OPTION | DESCRIPTION<br>Card No. | Columns | Contents |
|---|---|---|---|
| TITLE | Input a new title. If this option is not activated, the default title is "Standard Ozone Isopleth Conditions." | | |
| | 1 | 1-4 | TITL |
| | 2 | 1-72 | The title can be placed anywhere in card columns (cc) 1-72 |
| PLACE | Input city-specific information on light intensity. Default values correspond to Los Angeles on June 21, 1975. | | |
| | 1 | 1-4 | PLAC |
| | | 11-20 | Latitude, in decimal degrees north of the equator; DF = 34.058. |
| | | 21-30 | Longitude, in decimal degrees west of Greenwich meridian; DF = 118.250. |
| | | 31-40 | The time zone, in hours from Greenwich mean time; DF = 8.0. |
| | | 41-50 | The year; DF = 1975. |
| | | 51-60 | The month of year; DF = 6. |
| | | 61-70 | The numerical day of month; DF = 21. |
| | 2 (optional) | 1-24 | The name of the place can be entered anywhere in cc 1-24. Include this card only if a new value is entered for the latitude or longitude on the previous card. |

TABLE 4-1. (Cont'd)

INPUT FORMAT FOR OZIPP OPTIONS

| OPTION | | DESCRIPTION | |
|---|---|---|---|
| | Card No. | Columns | Contents |
| DILUTION | | Input city-specific information on inversion rise. | |
| | 1 | 1-4 | DILU |
| | | 11-20 | Initial inversion height, Z1, in any units; DF = 510. |
| | | 21-30 | Final inversion height, Z2, in same units as initial inversion height; DF = 630. |
| | | 31-40 | Starting time of inversion rise (24 hour daylight time); DF = 0800. |
| | | 41-50 | Ending time of inversion rise (24 hour daylight time); DF = 1500. |
| EMISSIONS | | Input city-specific information on post-0800 emissions. | |
| | 1 | 1-4 | EMIS |
| | | 11-20 | The number of hours for which emission fractions are to be input, from 1.0 to 10.0; DF = 0. This number should be coded as positive if the same fractions for NMHC and $NO_x$ are to be used. It should be coded as negative if different fractions are to be used. |
| | | 21-30 | NMHC or NMHC and $NO_x$ emission fraction for hour 1; DF = 0. If all NMHC fractions are to be set to zero, enter any negative number and skip to card 3. |
| | | 31-40 | NMHC or NMHC and $NO_x$ emission fraction for hour 2; DF = 0. |
| | | 41-50 | NMHC or NMHC and $NO_x$ emission fraction for hour 3; DF = 0. |

TABLE 4-1. (Cont'd)

INPUT FORMAT FOR OZIPP OPTIONS

| OPTION | DESCRIPTION | | |
|---|---|---|---|
| | Card No. | Columns | Contents |
| EMISSIONS (Cont'd) | | | |
| | | 51-60 | NMHC or NMHC and $NO_x$ emission fraction for hour 4; DF = 0. |
| | | 61-70 | NMHC or NMHC and $NO_x$ emission fraction for hour 5; DF = 0. |
| | 2*<br>(optional) | 1-10 | NMHC or NMHC and $NO_x$ emission fraction for hour 6; DF = 0. |
| | | 11-20 | NMHC or NMHC and $NO_x$ emission fraction for hour 7; DF = 0. |
| | | 21-30 | NMHC or NMHC and $NO_x$ emission fraction for hour 8; DF = 0. |
| | | 31-40 | NMHC or NMHC and $NO_x$ emission fraction for hour 9; DF = 0. |
| | | 41-50 | NMHC or NMHC and $NO_x$ emission fraction for hour 10; DF = 0. |
| | 3*<br>(optional) | 1-10 | $NO_x$ emission fraction for hour 1; DF = 0. If all $NO_x$ fractions are to be set to zero, enter any negative number in cc 1-10, skip card 4 and proceed to the next option. |
| | | 11-20 | $NO_x$ emission fraction for hour 2; DF = 0. |
| | | 21-30 | $NO_x$ emission fraction for hour 3; DF = 0. |
| | | 31-40 | $NO_x$ emission fraction for hour 4; DF = 0. |
| | | 41-50 | $NO_x$ emission fraction for hour 5; DF = 0. |
| | | 51-60 | $NO_x$ emission fraction for hour 6; DF = 0. |
| | | 61-70 | $NO_x$ emission fraction for hour 7; DF = 0. |

* See footnote on next page.

TABLE 4-1 (Cont'd)

INPUT FORMAT FOR OZIPP OPTIONS

| OPTION | DESCRIPTION Card No. | Columns | Contents |
|---|---|---|---|
| EMISSIONS (Cont'd) | | | |
| | 4* | 1-10 | $NO_x$ emission fraction for hour 8; $DF^x = 0$. |
| | (optional) | 11-20 | $NO_x$ emission fraction for hour 9; $DF^x = 0$. |
| | | 21-30 | $NO_x$ emission fraction for hour 10; $DF^x = 0$. |

---

* Card 2 is not included if there are less than 5 hours of emissions or if all individual NMHC fractions were set to zero by entering a negative number in cc 21-30 of Card 1. Cards 3 and 4 are not included if combined NMHC and $NO_x$ fractions were entered in Cards 1 and 2. Card 4 is not included if all individual $NO_x$ fractions were set to zero by entering a negative number in cc 1-10 of Card 3, or if there are less than 8 hours of $NO_x$ emissions.

## TABLE 4-1 (Cont'd)

## INPUT FORMAT FOR OZIPP OPTIONS

| OPTION | | DESCRIPTION | |
|---|---|---|---|
| | Card No. | Columns | Contents |
| REACTIVITY | | Input city-specific information on reactivity. | |
| | 1 | 1-4 | REAC |
| | | 11-20 | Initial fraction of carbon atoms in the form of propylene; DF = 0.25. |
| | | 21-30 | Initial $NO_2/NO_x$ ratio; DF = 0.25. |
| | | 31-40 | Fraction of initial NMHC concentration (in ppmC) added as aldehyde; DF = 0.05. |
| TRANSPORT | | Input city-specific information on transported pollutants. | |
| | 1 | 1-4 | TRAN |
| | | 11-20 | Concentration of $O_3$ transported in the surface layer, in ppm; DF = 0. |
| | | 21-30 | Concentration of $O_3$ transported aloft, in ppm; DF = 0. |
| | | 31-40 | Concentration of NMHC transported in the surface layer, in ppmC; DF = 0. |
| | | 41-50 | Concentration of NMHC transported aloft, in ppmC; DF = 0. |
| | | 51-60 | Concentration of $NO_x$ transported in the surface layer, in ppm; DF = 0. |
| | | 61-70 | Concentration of $NO_x$ transported aloft, in ppm; DF = 0. |

TABLE 4-1 (Cont'd)

INPUT FORMAT FOR OZIPP OPTIONS

| OPTION | | DESCRIPTION | |
|---|---|---|---|
| | Card No. | Columns | Contents |
| ACCURACY | | Increase or reduce the mathematical accuracy of the isopleth diagram by using more or fewer simulations, more or less accurate interpolation, etc. | |
| | 1 | 1-4 | ACCU |
| | | 11-20 | Number of constant initial NMHC/$NO_x$ ratios (radial lines from the origin of the isopleth diagram) on which simulations are to be performed, any odd number from 1. to 19.; DF = 11. |
| | | 21-30 | Number of simulations per radial line, from 1. to 8.; DF = 5. |
| | | 31-40 | Error tolerance in the numerical integration routine, from 0.1 to 0.00001; DF = 0.01. |
| | | 41-50 | Tension factor for hyperbolic spline functions used in first stage of interpolation from .001 to 50.; DF = 1. |
| | | 51-60 | Tension factor for hyperbolic spline functions used in plotting isopleth lines (high tensions lead to straight lines drawn between the points obtained from the first stage), from .001 to 50.; DF = 1. |
| | | 61-70 | If any non-zero value is entered in this field, simulations will terminate after any ozone maximum; no entry produces full 10-hour simulations. |

## TABLE 4-1 (Cont'd)
## INPUT FORMAT FOR OZIPP OPTIONS

| OPTION | DESCRIPTION<br>Card No. | Columns | Contents |
|---|---|---|---|
| ALREADY | | Include results from a previous run. | |
| | 1 | 1-4 | ALRE |
| | | 11-20 | Number of previous simulations to be input. |
| | 2* | 1-10 | Initial NMHC concentration, ppmC |
| | | 11-20 | Initial $NO_x$ concentration, ppm. |
| | | 21-30 | Maximum one-hour average ozone concentration, ppm. |

---

* One card is included for each simulation result. Thus, the number of these cards must be equal to the value coded in cc 11-20 of Card 1. Also, the cards must be put in the same order in which the simulations were performed.

TABLE 4-1 (Cont'd)

INPUT FORMAT FOR OZIPP OPTIONS

| OPTION | DESCRIPTION<br>Card No. | Columns | Contents |
|---|---|---|---|
| PLOT | Activates the drawing of the isopleth diagram on an offline plotter | | |
| | 1 | 1-4 | PLOT |
| | | 11-20 | Scaling factor for the location of labels for each ozone isopleth. The value should be between 0.1 and 0.8.; DF = 0.6. |
| | | 21-30 | If non-zero, a grid is overlaid on the diagram. If the value is positive and non-zero, a grid is overlaid on the diagram using a different color pen (if available).<br>If the value is negative, a grid with lines of different patterns (e.g., dot-dash) is overlaid on the plot. The absolute value of this number corresponds to different patterns and texture. |
| | | 31-40 | Length (in inches) of the abscissa (NMHC scale) of the isopleth diagram; DF = 8.5. |
| | | 41-50 | Length (in inches) of the ordinate ($NO_x$ scale) of the isopleth diagram; DF = 5.95. |
| | | 51-60 | Sizes (in inches) of the numbers to be printed on the axes and of the characters in the title; DF = 0.10. |
| | | 61-70 | The sizes (in inches) of the labels on the ozone isopleths and the division marks on the axis; DF = 0.07. |

## TABLE 4-1 (Cont'd)

## INPUT FORMAT FOR OZIPP OPTIONS

| OPTION | Card No. | DESCRIPTION<br>Columns | Contents |
|---|---|---|---|
| CALCULATE | | Perform a single simulation with the initial NMHC and $NO_x$ concentrations specified on this card. | |
| | 1 | 1-4 | CALC |
| | | 11-20 | Initial NMHC concentration in ppmC. |
| | | 21-30 | Initial $NO_x$ concentration in ppm. |
| | | 31-40 | Information option; entry of any positive value will result in printing of the computed concentrations of all species, the rates of change of all species, reaction rates, etc. Photolysis constants are also printed. |
| | | 41-50 | Time (in minutes) from the beginning of the simulation at which computed concentrations of all species in the kinetic mechanism are to be printed; DF = 60. |
| | | 51-60 | Time step (in minutes) for subsequent printing of concentrations; DF = 60. |

TABLE 4-1 (Cont'd)

INPUT FORMAT FOR OZIPP OPTIONS

| OPTION | DESCRIPTION<br>Card No. | Columns | Contents |
|---|---|---|---|
| ISOPLETH | | | Construct an ozone isopleth diagram according to the input parameters. Default isopleths are 0.08, 0.12, 0.16, 0.20, 0.24, 0.28, 0.30, 0.32, 0.34, 0.36 and 0.40 ppm. |
| | 1 | 1-4 | ISOP |
| | | 11-20 | Maximum NMHC concentration (in ppmC) on abscissa of isopleth diagram; DF = 2.0. |
| | | 21-30 | Maximum $NO_x$ concentration (in ppm) on ordinate of isopleth diagram; DF = 0.28. |
| | | 31-40 | Number of ozone isopleths to be drawn, from 1. to 20.; DF = 11. |
| | | 41-50 | Any non-zero value will activate the printing of solar noon and the time of the center of the maximum one-hour average ozone concentration for each simulation. |
| | 2*<br>(optional) | 1-10 | Ozone concentration of 1st isopleth, ppm; |
| | | 11-20 | Ozone concentration of 2nd isopleth, ppm; |
| | | 21-30 | Ozone concentration of 3rd isopleth, ppm; |
| | | 31-40 | Ozone concentration of 4th isopleth, ppm; |
| | | 41-50 | Ozone concentration of 5th isopleth, ppm; |
| | | 51-60 | Ozone concentration of 6th isopleth, ppm; |
| | | 61-70 | Ozone concentration of 7th isopleth, ppm. |

* See footnote on next page.

## TABLE 4-1 (Cont'd)
## INPUT FORMAT FOR OZIPP OPTIONS

| OPTION | DESCRIPTION | | |
|---|---|---|---|
| | Card No. | Columns | Contents |
| | 3*<br>(optional) | 1-10 | Ozone concentration of 8th isopleth, ppm. |
| | | . | . |
| | | . | . |
| | | . | . |
| | | 61-70 | Ozone concentration of 14th isopleth, ppm. |
| | 4*<br>(optional) | 1-10 | Ozone concentration of 15th isopleth, ppm. |
| | | . | . |
| | | . | . |
| | | . | . |
| | | . | . |
| | | 51-60 | Ozone concentration of 20th isopleth, ppm. |
| bbbb | | A blank card must follow all input cards to terminate the program. | |
| | 1 | 1-4 | Blanks. |

* Optional cards 2,3, and 4 are input only if the number of isopleths to be drawn is specified on Card 1. The number of entries, and thus the number of optional cards, must correspond to the number of isopleths to be drawn. For example, if 10 isopleths are specified, entries are made in the first 7 fields of Card 2 and the first 3 fields of Card 3. Card 4 would not be included with the input. Note that the default scheme does not apply when an entry is made in Columns 31-40 of the first card (i.e., the ISOP card).

## 4.2 PROGRAM GENERATED ERROR MESSAGES

This section discusses potential output error messages produced by OZIPP. Two types or error messages are generated:

- Fatal error messages -- messages caused by problems that immediately halt any further computation.
- Non-Fatal error messages--messages caused by problems that do not cause an immediate halt in computation.

These types of messages are discussed below.

### 4.2.1 Fatal Error Messages

There are seven fatal error messages that may occur during OZIPP runs. Five of these occur because the integration scheme cannot proceed further. Descriptions of each message are included below:

- THE LOWEST OZONE LINE CANNOT BE PLOTTED
  INCREASE THE MAXIMUM HC AND $NO_x$ VALUES

  If the concentration of ozone predicted from the maximum initial NMHC and $NO_x$ concentrations (listed on the ISOPLETH card, or NMHC = 2.0 ppmC, $NO_x$ = 0.28 ppm by default) is less than the lowest ozone isopleth line to be plotted, the program will stop. The user may fix this problem by either increasing the maximum NMHC or $NO_x$ concentrations or reducing the concentrations at which ozone isopleths are to be plotted.

- NO LINES CAN BE PLOTTED
  BACKGROUND ONLY PRODUCES TOO MUCH OZONE ____ PPM

  This message is the opposite of the previous message. If the amount of ozone predicted at NMHC and $NO_x$ concentrations of 0.0 is greater than the highest ozone isopleth line desired, the program will stop.

The following error messages all stem from problems encountered in the integration scheme routines:

- PROBLEM APPEARS UNSOLVABLE WITH GIVEN INPUT

- INTEGRATION HALTED BY DRIVER AT T = ____
  EPS TOO SMALL TO BE ATTAINED FOR THE MACHINE PRECISION

- KFLAG = -2 FROM INTEGRATOR AT T = ____, H = ____
  THE REQUESTED ERROR IS SMALLER THAN CAN BE HANDLED

- KFLAG = -3 FROM INTEGRATOR AT T = ____
  CORRECTOR CONVERGENCE COULD NOT BE ACHIEVED

- ILLEGAL INPUT..EPS.LE.0.

If any of these messages occur, the user should try the following:

- Check input to be sure all data are correct (e.g., check hydrocarbon and $NO_x$ values on a CALCULATE option, check for negative error tolerance, and so on).

- Raise the value of the error tolerance, if necessary.

- Redefine the density of simulations (e.g., change the number of radials, number of simulations per line, maximum initial NMHC or $NO_x$ concentrations, etc.)

- As a last resort, alter the simulation conditions slightly (e.g., change post-0800 emissions, dilution, etc.)

### 4.2.2 Non-fatal Error Messages

Two non-fatal error messages may occur in OZIPP runs. The user may wish to redefine the situation (i.e., the limits of the diagram) or to check the input data.

- THE OPTIONS INSTRUCTION__CANNOT BE PROCESSED

  If this message occurs, the user should check for an error in the input data.

- DUE TO HIGH BACKGROUND CONDITIONS
  THE LOWEST OZONE PLOTTED WILL BE ____PPM

  This message indicates that some of the ozone isopleths desired lie outside the limits of the diagram. For example, if the maximum ozone concentration associated with zero initial conditions were greater than 0.08 ppm, a 0.08 ppm isopleth could not be drawn. However, isopleths greater than 0.08 ppm could possibly be drawn.

## 4.3 COMPUTER CONSIDERATIONS

The OZIPP program consists of one main program and 39 subprograms. It requires about 41K, 36-BIT words of core in a UNIVAC-1110 computer system. Run times on the system average 5-7 minutes. Complete listings, along with flow diagrams of selected subroutines, are shown in Appendices B and C, respectively. Also included are five calls to CALCOMP subroutines. Discussed below are special language considerations, use of CALCOMP routines and computer control language.

### 4.3.1 Language Considerations

Although OZIPP has been written to conform with ANSI standard FORTRAN language, there are certain types of language usage in OZIPP that are not compatible on all computer systems. Areas to check include the following multiple-entry points:

| | |
|---|---|
| ·Subroutine DIFFUN | card(L.1) |
| entry point: | |
| ENTRY DIFSET(...) | card(L.71) |
| ·Subroutine ISOPLT | card(V.1) |
| 2 entry points: | |
| ENTRY SAVLIN(...) | card(V.77) |
| ENTRY LINPRT(...) | card(V.93) |
| ·Subroutine VVLBLF | card(AL.1) |
| 2 entry points: | |
| ENTRY VVLBLC(...) | card(AL.60) |
| ENTRY VVLBLL(...) | card(AL.165) |

These entry points may or may not require the argument list after the ENTRY statement.

The variable UROUND in subroutine DRIVES should be set to the round-off error associated with each computer system. Currently, UROUND is set to the round-off error of $7.5 \times 10^{-9}$ associated with a UNIVAC 1110 computer system. To reset UROUND, the card (J.12) in subroutine DRIVES should be changed:

·DATA     UROUND/user's round-off error/     (card J.12)

UROUND is calculated from the number of significant digits (N) used for the mantissa of a floating point constant:

$$\text{UROUND} = 2^{-N}$$

For the UNIVAC 1110 computer, each word contains 36-BITs of which 27 are used for the mantissa. Thus, $2^{-27}$ is equal to approximately $7.5 \times 10^{-9}$. This is the value currently set in OZIPP.

Another variable in OZIPP which is machine dependent is the variable EXPMAX found in subroutines CURV1 and KURV1. This variable represents the maximum possible value for the exponent of e. For the UNIVAC 1110 computer, the range of the real constants is from $10^{-38}$ to $10^{38}$. Hence, the maximum value for the exponent of e:

$$e^{\text{EXPMAX}} = 10^{38}$$

or EXPMAX is 87.5 for the UNIVAC 1110 computer. The value currently set in OZIPP is 87.4, which is slightly lower than the actual maximum value to ensure that the actual maximum is never reached. To reset EXPMAX, the user must change the cards (W.43 and Y.45A) accordingly:

```
            DATA EXPMAX/user's maximum exponent/          W.43
    and     DATA EXPMAX/user's maximum exponent/          Y.45A
```

### 4.3.2 Use of CALCOMP Routines

The CALCOMP routines required by OZIPP are:

```
·Subroutine PLOT (XX,YY,IX)
     "      PLOTS (XX,YY,IX)
     "      SYMBOL (XX,YY,HT,ITX,ANG,NCH)
     "      NUMBER (XX,YY,HT,FPN,ANG,NDEC)
     "      NEWPEN (IPEN)
```

For users without access to these CALCOMP routines, dummy routines may be needed in order to run OZIPP. To generate the dummy routines, the user must have the following cards for each of the above routines:

```
·SUBROUTINE______(argument list)

·RETURN

·END
```

For users with standard CALCOMP routines, no modifications to OZIPP are required. The user should check that the five routines have the same names in their system as given above.

### 4.3.3 Control Language

The following runstream illustrates the Executive Control Language (ECL) necessary to execute the OZIPP program on a UNIVAC 1110 computer system:

```
@RUN,   priority, job, account, userid, time
@ASG,A  prog-file
@PLOT   plotfile.
@XQT    prog-file.abselement
card input deck
@FREE   PLOTFILE.
@SYM    PLOTFILE.,,PLOT
@FIN
```

where:

priority = job priority

jobid = six-character job identification

account = user account number

userid = user identification code

time = time requirement for executing the job

prog-file = name of program file containing the OZIPP absolute element

plotfile = a CALCOMP-produced file that contains the controls for constructing the plot on an off-line plotter

card input deck = the input option cards

Note that the job control language will be different for most computer systems, but the basic requirements for running OZIPP are the same.

## 5.0 EXAMPLE OZIPP RUNS

In this chapter, examples demonstrating the routine functioning of OZIPP are presented. The procedures for obtaining both the standard ozone isopleth diagram and city-specific diagram are illustrated. Input and output data for each type of run are described. These examples can be used as installation test cases. Because of the internal precision associated with various computer systems, comparisons between results obtained using two different computing systems may show slight numerical differences. However, these differences should not exceed one percent.

One important application of the city-specific OZIPP is to estimate control requirements for the case in which transported pollutant concentrations in the future are expected to be reduced. An example of how OZIPP is used with the EKMA technique for this situation is presented in Section 5.3.

OZIPP was designed to handle a wide variety of isopleth diagrams, but there may be some sets of conditions that cause unusual plots (e.g., wavy isopleths, uneven spacing of isopleths, etc.) In some cases, such plots can be modified by altering the tension factor. This is illustrated in Section 5.4.

### 5.1 THE STANDARD OZONE ISOPLETH DIAGRAM

The standard ozone isopleth diagram is produced by using all default values as input. Sixty-two simulations are performed in all, with 5 simulations performed on each of eleven radials. Seven additional simulations are performed as described in Section 2.3.

#### 5.1.1 Input Data For Standard Diagram Example

Because all input data are set to default conditions to produce the standard ozone isopleth diagram, only one option needs to be activated - the ISOPLETH option. However, in this example, it is assumed that a CALCOMP plot of the standard diagram is also to be produced, with a grid system overlaid on the diagram. Figure 5-1 shows the input data necessary to produce such a standard diagram.

FIGURE 5-1. INPUT DATA FOR STANDARD OZONE ISOPLETH DIAGRAM EXAMPLE

```
PLOT              1.0      5.1      3.6      0.06     .042
ISOP
blank card
```

The PLOT option activates the off-line plotting software. The "1.0" is entered in the second numeric field on that card (i.e., Columns 21-30). This parameter causes gridded lines of different color to be overlaid on the diagram. If no overlay is desired, the "1.0" should not be entered on the card. The remaining parameters on the PLOT card set the lengths of the abscissa and ordinate, the size of the characters, and the size of the labels. (The size of the plot produced with these parameters is roughly 60 percent of the size produced with default values). If only a line-printer plot is desired, the PLOT option card should be removed from the input data.

The ISOPLETH card causes OZIPP to perform the sixty-two simulations with default simulation conditions (since no default conditions were overridden except for the PLOT option) and to produce the standard ozone isopleth diagram. The blank card at the end of the input deck is required for all runs. It terminates the program after processing all options.

### 5.1.2 Program Output For Standard Diagram Example

The output for the standard diagram run is presented in Appendix D. The output from this run consists of three parts. The first part contains a header page describing the conditions used for the simulations. Assumptions about location, time of year, dilution and reactivity are all summarized.

The second part of the output presents the simulation results. For each simulation, the initial NMHC and $NO_x$ concentration, the initial NMHC/$NO_x$ ratio and the calculated maximum one-hour average ozone concentration are printed. In some simulations, the ozone concentration rises throughout the 10-hour simulation period. If this condition is encountered in a simulation, "NOT MAX" is printed next to the ozone value.

The final part of the output is the ozone isopleth diagram. A line-printer plot is always produced. The off-line diagram produced as a result of activating the PLOT option is also shown in Appendix D.

## 5.2 EXAMPLE CITY-SPECIFIC DIAGRAM

In developing a city-specific isopleth diagram, there are two important factors to consider. The first involves estimating city-specific parameters (such as emissions, dilution and transport conditions) that are representative of the city of interest. The second involves setting the other OZIPP input parameters so that a diagram is obtained which is suitable for use with the EKMA method. In this section, procedures for addressing both of these problems are illustrated through the use of an example problem.

### 5.2.1 Determination of City-Specific Parameters

The assumptions made for the city-specific parameters used in the example problem are described below. The primary guide to be used in formulating these parameters for any particular city is Appendix B of Reference 1. Some of the information presented in Reference 1 has been repeated here to illustrate the procedures to be used in developing city-specific information.

#### A. Light Intensity Data

The OZIPP model requires information on city location and day of the year to calculate the diurnal variation of photolytic rate constants. Latitude and longitude for city center are used to specify the city location. The date used should be the day on which the design ozone concentration occurs. (The design value of ozone is normally defined as the highest second-high hourly ozone concentration measured in or near a city. The reader is referred to Reference 1 for more details.) For the example problem, a latitude of 39.0 and a longitude of 77.0 were selected. Because this latitude and longitude fall in the Eastern Time Zone, the Numerical Time Zone of 5.0 corresponding to Eastern Daylight Time was chosen (see Section 3.2.1). The design ozone concentration was assumed to have been measured on August 1, 1977.

#### B. Dilution Data

To account for dilution effects, the OZIPP model requires data on a minimum mixing height, a maximum mixing height, the time at which the mixing height rise begins and the time at which it ends. Ideally, these data should be based on observations taken on the day being modeled. However, it is usually necessary to use some other indicators of these data. For example, a suitable surrogate for the design day data is median data based on days with high ozone levels. Often, the only data available are seasonal mean morning and afternoon mixing heights as provided in Reference 10. If no local information is available on the time of day during which the mixing height is increasing, it may be assumed that increases in mixing height typically occur between 0800 and 1500 LDT. For the example problem, data from Reference 10 for the Washington, D. C. area were used. The morning mixing height was assumed to be 425 meters, and the afternoon height 1900 meters. The mixing height rise was assumed to take place over a seven hour period beginning at 0800 LDT.

### C. Post-0800 Emissions Data

If it is desired to include the effects of post-0800 emissions, information on relative emission rates must be input. Relative emission rates express the rate of emissions injected into the imaginary column of air for each hour of simulation relative to emissions into the air column prior to the 0800 LDT simulation starting time. The emissions prior to 0800 are represented by the initial NMHC and $NO_x$ concentrations. Post-0800 emissions are represented by additions to these precursor concentrations.

Relative emission rates are required for each hour of simulation. A rigorous calculation would require a precise specification of: (1) the location of the column, (2) the spatial variation in emissions and (3) the temporal variation in emissions. Unfortunately, these data are not often available and the task then becomes one of deriving reasonable approximations with the data that are available. The most practical approach is then to roughly approximate the spatial and temporal variations in emissions along a hypothetical column trajectory. One such approach is described below. However, the assumptions and values discussed below are included primarily for illustrative purposes. City-specific information should be used wherever possible.

An estimation of relative emission rates may be made assuming column trajectories that move from the center of the city to the urban limit. As the column moves away from the center of the city, emissions into it typically decrease. One formulation that can be used to depict the decrease of emissions with distance from the center of the city is:

$$e_s = Q_0 \exp(-ax^2)$$

where

$e_s$ = emissions at location s

$Q_0$ = the emissions in the center of the city

a = constant (may relate to the wind speed or speed at which the column is moving)

x = the distance the column has moved from the center of the city

This spatial pattern is in the form of a Gaussian distribution as discussed in Reference 1. (Other types of distributions may be postulated.) For the example problem, the spatial distribution of emissions was determined using the same assumptions as used in Reference 1: (1) the column leaves the center of the city at 0800 LDT and moves at constant velocity until it leaves the urban area three hours later; and (2) the emissions at the edge of the urban area are $e^{-2}$ (approximately 0.14) of the emissions in the center of the city. An estimate of the average emissions for each hour was made by calculating the emissions at the mid-point of each hour (e.g., 0830 for the hour from 0800 to 0900). The second column of Table 5-1 shows the results of these calculations. These spatial adjustment factors are the hourly factors expressing the emissions at the location of the column relative to the emissions in the center city.

After the spatial distribution of emissions has been determined, the temporal distribution is required. In the absence of site-specific information, a city-wide average may be used. This distribution may be calculated as

TABLE 5-1. EXAMPLE OF ESTIMATION OF EMISSIONS FRACTIONS FOR OZIPP

| Time (LDT) | Spatial Adjustment | | Percent of Day's Emissions | | Composite Relative Emission Rate (percent) | Normalized Relative Emission fraction* |
|---|---|---|---|---|---|---|
| 12 - 8 a.m. | 1.0 | x | 16.9 | = | 16.9 | 1.0 |
| 8 - 9 a.m. | 0.95 | x | 6.4 | = | 6.1 | .36 |
| 9 - 10 a.m. | 0.61 | x | 4.4 | = | 2.7 | .16 |
| 10 - 11 a.m. | 0.25 | x | 4.8 | = | 1.2 | .07 |
| after 11 a.m. | negligible | | --- | | negligible | negligible |

* The composite relative emission rate normalized relative to the 0800 composite rate. These are the input values for OZIPP.

Source: Reference 1.

the average of the temporal distribution of mobile and stationary sources. In some cases, the temporal distribution of automotive emissions may be an adequate representation of the temporal distribution of the total emissions. The distribution used for the example problem was taken from Reference 1, and is shown in the third column of Table 5-1.

To obtain the relative emissions for input to OZIPP, the spatial and temporal factors are multiplied and then normalized to the initial emissions. These processes are presented in Columns 4 and 5 in Table 5-1. The fractions in the last column were used as input for the example problem.

### D. Transported Pollutant Data

For a detailed discussion of pollutant transport as it relates to EKMA, the reader is referred to Reference 1. Normally, estimates of pollutants transported into the area of interest are based on measurements taken upwind of the city. Recall that transport of three types of pollutants (NMHC, $NO_x$ and ozone) can be considered in two layers - the surface layer and the air above the base of a nocturnal inversion layer. For the example problem, it was assumed that ozone was transported aloft with a concentration of 0.10 ppm. The concentrations of the other pollutants were assumed negligible.

### E. Reactivity Data

In Reference 1, it is recommended that the default reactivity factors not be altered. This recommendation is based on two premises:

1) sensitivity studies have indicated that the maximum calculated ozone concentration is relatively insensitive to the $NO_2/NO_x$ mix, and

2) limited knowledge exists about the mix of organic species in urban areas and it is very difficult to estimate the equivalent combination of propylene and n-butane.

For the example run, all reactivity factors, consequently, were left at the default values.

### 5.2.2 Diagram Definition

The basic data needed to use an ozone isopleth diagram with EKMA are an NMHC/$NO_x$ ratio and an observed one-hour average ozone concentration. The optimal diagram arrangement is one in which the observed NMHC/$NO_x$ ratio is near the diagonal of the diagram and the ozone isopleth corresponding to the observed ozone design value is in the upper right quadrant of the diagram. The isopleth lines should be fairly evenly spaced and spread across the diagram, rather than in one corner or along an edge. Even spacing and coverage provides optimal utilization of the OZIPP algorithm.

The basic procedure recommended for determining the appropriate maximum NMHC and $NO_x$ initial concentrations and the isopleth levels for the diagram is one of trial and error. It should be remembered that all isopleth diagrams in OZIPP are plotted with 10 horizontal scale divisions and 7 vertical ones. Consequently, it may be advisable to choose an $NO_x$ maximum evenly divisable by 7. One way to test for the appropriate scale is to use the CALCULATE option to calculate the maximum ozone concentrations associated with potential NMHC and $NO_x$ diagram maxima. The combination of NMHC and $NO_x$ maxima to use in the run creating the diagram is one which will result in the ozone design value being located in the upper right quadrant of the diagram. The concentrations for the isopleths may be altered from the default values, depending on the calculated maximum ozone concentration. For example, if the calculated maximum ozone concentration were 0.20 ppm, isopleth values much greater than this could be replaced with lower values in order to obtain better diagram resolution.

The above procedure can be illustrated with the example problem. Assume that the design NMHC/$NO_x$ ratio is 5.0 and the design ozone concentration is 0.16 ppm. A single OZIPP run was made using multiple CALCULATE options to test possible NMHC and $NO_x$ maxima. Because the $NO_x$ scale is divided into seven equal increments, the $NO_x$ values selected were all even multiples of 0.07. (Using one of these values will produce a graph that is easy to read.) The NMHC value corresponding to each of the potential $NO_x$ maxima was chosen such that the NMHC/NO$_x$ ratio was approximately equal to the design value and the NMHC scale would be easy to read. The results of the simulations performed to test the maxima are summarized below:

| NO$_x$ | NMHC | NMHC/NO$_x$ | Maximum Ozone |
|---|---|---|---|
| .42 | 2.0 | 4.8 | .30 |
| .35 | 1.8 | 5.1 | .28 |
| .28 | 1.5 | 5.4 | .25 |
| .21 | 1.0 | 4.8 | .21 |
| .14 | 0.7 | 5.0 | .17 |

The maxima selected for use in producing the isopleth diagram were 0.21 and 1.0 for NO$_x$ and NMHC, respectively. These values will result in the design ozone concentration being located in the upper right quadrant of the diagram.

### 5.2.3 Input Data For City-specific Example

The input data for the example city-specific run are shown in Figure 5-2. Several options have been included for illustrative purposes. The input data are set up to perform two single simulations and then to construct an isopleth diagram using the ISOPLETH option.

The first option causes the default title to be replaced by the title on the next card, i.e., "CITY-SPECIFIC EXAMPLE". All output is labeled with this title.

The PLACE option is used to override the default location and day of year. The first two numeric fields contain the latitude and longitude for the example city. The next numeric field contains the time zone indicator. The city is assumed to be in the Eastern Time Zone, so 5.0 is entered as the numerical time zone (see Section 3.2.1). The next three fields contain the year, month and day - August 1, 1977. The card following the PLACE option contains the name of the example city.

## FIGURE 5-2. INPUT DATA FOR CITY-SPECIFIC DIAGRAM EXAMPLE

```
TITL
CITY-SPECIFIC EXAMPLE
PLAC          39.0         77.0       5.          1977.       8.        .1.
TEST RUN CITY
DILU         425.0       1900.0
EMIS           3.0          0.36      0.16           0.07
TRAN                        0.10
ALRE           4.
0.0            0.0           .06229
0.0            0.14          .04664
0.7            0.14          .17315
0.7            0.0           .06774
PLOT                                  5.1            3.6      0.08      0.06
CALC           1.0          0.21
CALC           1.0          0.21      1.0
ISOP           0.7          0.14      6.0            1.0
.06             .08          .10      0.12           0.14     0.16
blank card
```

The data on dilution is entered by using the DILUTION option card. The morning and afternoon mixing heights are entered in the first two numeric fields. Because no other entries are made on this card, the starting time and ending time of the inversion rise will remain at default values, namely 0800 and 1500 LDT, respectively.

The emissions data are entered via the EMISSIONS option card. The first numeric field indicates that emissions data are input for the first three hours of the simulation. The next three numeric fields contain the relative emission fractions. Note that, because the number of hours coded in the second numeric field is positive, the relative emission fractions apply to both NMHC and $NO_x$.

The TRANSPORT option card is used to enter the data on transported pollutant concentrations. The concentration of ozone transported aloft (0.10 ppm) is input in the second numeric field. Because all other fields are left blank, the concentrations of all other transported pollutants remain at default levels (i.e., zero).

The ALREADY option has been included simply to illustrate its use. The 4.0 entered in the first numeric field indicates that the results of 4 simulations are to be input. Note that these simulations must be input in the order that they would normally occur in the run, starting with the first. (In other words, if there are 10 input simulations, they must be the 1st through the 10th). The 4 cards following the ALREADY option contain the previous simulation results. On each card, the first field (i.e., Columns 1-10) contains the initial NMHC concentration, the second field the initial $NO_x$ concentration, and the third field the maximum-one-hour ozone concentration.

The PLOT option activates the off-line plotting software. The lengths of the abscissas and ordinate of the diagram are set to 5.0 inches and 3.6 inches by the entries in the third and fourth numeric fields of this card. The other parameters control the size of the characters and labels on the graph.

The first CALCULATE option results in one particular simulation being performed with initial NMHC and $NO_x$ concentrations of 1.0 ppmC and 0.21 ppm, respectively. The second CALCULATE option produces the same simulation. In this case, however, the information option is activated by entering "1.0" in the third numeric field. The detailed information is to be printed for hourly intervals because the fourth and fifth numeric fields have been left blank and the default values are used (see Table 4-1).

The final option, ISOPLETH, causes an ozone isopleth diagram to be produced. The first two numeric fields contain the maximum NMHC and $NO_x$ initial concentrations for the diagram (0.7 ppmC and 0.14 ppm, respectively). The 6.0 coded in the third numeric field indicates that 6 isopleths are to be drawn on the diagram. The isopleth levels themselves are entered on the next two cards. The positive number coded in the fourth numeric field activates the printing of solar noon and the time of the center of the maximum one-hour average ozone concentration.

Again, note that the ordering of the option cards is unimportant, except that the ISOPLETH and CALCULATE cards must come after all other options have been activated. Data cards (i.e., those without a code word in the first field) must be in the order specified in Table 4-1. Also, default values will be assumed for any numeric field left blank.

### 5.2.4 Program Output For City-specific Example

Appendix E contains all the program output for the city-specific example. First, the ALREADY option causes the input simulation results to be reprinted in tabular form. The first CALCULATE option produces three pages of output. The first page is a tabular summary of the simulation conditions. The second table gives instantaneous pollutant concentrations at hourly intervals. The maximum one-hour average ozone concentration is printed at the bottom of the table. The last page of output produced by this option is a graph of instantaneous ozone concentration versus time.

The second CALCULATE card has the informtion option activated and thus produces much more output. First, the table summarizing the simulation conditions is produced. A table is then printed giving the rate constants for each of the 76 reactions. Thirdly, a set of tables produces information on the instantaneous concentrations of all reactant species, their net rates of change, and the rates of all 76 reactions. For the example problem, such a table is produced at each hour of the simulation. Finally, a graph of ozone versus time is printed.

The ISOPLETH option produces three types of output. As with the CALCULATE option, a table summarizing the simulation conditions is first produced. Next, the results of each simulation are presented in tabular form. Note that the first simulation called for by the ISOPLETH option begins at the point where the simulations from the previous run ended (i.e., those entered using the ALREADY option). Finally, a line-printed plot of the ozone isopleth diagram is printed. Activation of the PLOT option along with the ISOPLETH option results in the off-line plot reproduced in Appendix E.

The conditions that produced this isopleth diagram led to some wiggles in the isopleth lines. The explanation for these wiggles is that these conditions produce two ozone peaks in the simulations. The first typically occurs after about 400 minutes of simulation, and the second near the termination of the simulation at 600 minutes. For low NMHC/$NO_x$ ratios (the upper part of the isopleth diagram), the first maximum is always smaller than the second. But for high NMHC/$NO_x$ ratios, the first maximum is larger. Near the diagonal, the two maxima are nearly equal. Thus, the isopleth diagram is really two diagrams superimposed. The area just above the diagonal is where the "first-peak" diagram is joined to the "second-peak" diagram.

This conclusion was reached after performing several simulations near the wiggles to ensure that these wiggles are not artifacts of interpolation. Another diagram for the same conditions, but with more calculations using the ACCURACY option, showed the same wiggles.

## 5.3 EXAMPLE TRANSPORT PROBLEM

An important application of the city-specific OZIPP is to estimate emission control requirements for the case in which future transported pollutant concentrations will be significantly different from current levels. Such a situation might occur as a result of the imposition of control measures upwind of the city of interest. The procedure of using OZIPP with the EKMA technique for this case is explained fully in Reference 1. An example transport problem is presented below to illustrate the technique.

For the example problem presented in Section 5.2, it was assumed that the concentration of ozone transported aloft was 0.10 ppm. It was also assumed that the design ozone value was 0.16 ppm and the design NMHC/$NO_x$ ratio was 5.0. For the example transport problem, the following additional assumptions will be made:

1) $NO_x$ concentrations will remain unchanged
2) ozone transported aloft will be reduced from 0.10 to 0.04 ppm
3) the air quality goal is 0.08 ppm.

The problem is then to estimate the reduction in NMHC concentrations required to meet the air quality goal.

The first step in the EKMA procedure is to generate the ozone isopleth diagram for the existing situation (i.e., 0.10 ppm ozone transported aloft). This is demonstrated in Section 5.2, and the diagram is shown in Figure E-3. The next step is to generate the isopleth for the air quality goal (i.e., 0.08 ppm) incorporating the assumption about future transported concentrations. This is accomplished by modifying only the TRANSPORT and ISOPLETH options of the input data that were used in the example problem in Section 5.2. The ozone transported aloft is changed from 0.10 to 0.04 ppm. The ISOPLETH option is modified to plot only the 0.08 ppm isopleth. The diagram generated by OZIPP with these modifications is shown in Figure 5-3.

The EKMA technique can now be applied to the problem. (For details of this procedure, see Reference 1.) The base initial NMHC and $NO_x$ concentrations are determined by using the base case diagram (Figure E-3), the design ozone

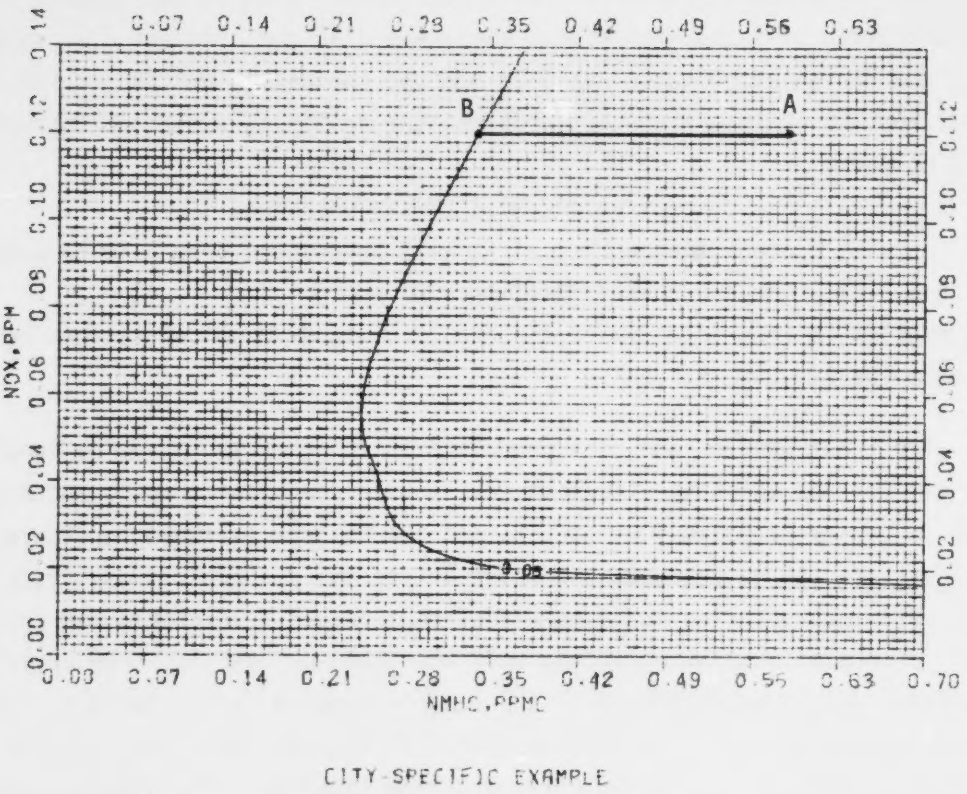

FIGURE 5-3. Example City-specific Diagram for Reduced Transport Case.

value and the NMHC/$NO_x$ ratio. For this problem, the base initial NMHC concentration is .60 ppmC, and the base initial $NO_x$ concentration is 0.12 ppm. This coordinate is then plotted on the new diagram (Point A on Figure 5-3). The NMHC reduction necessary to achieve the air quality goal is then represented by the line AB on Figure 5-3 (i.e., NMHC concentrations must be reduced from 0.6 ppmC to 0.34 ppmC, amounting to a NMHC reduction of 43 %).

## 5.4 USE OF THE TENSION FACTORS

In certain instances the user may have to plot ozone isopleths relatively close together on a large diagram. For example, a user may wish to plot isopleths at 0.10, 0.11 and 0.12 ppm on an isopleth diagram that has large maximum initial NMHC and $NO_x$ concentrations. This may cause the isopleths to be squeezed close together. An example of such an isopleth is shown in Figure 5-4. Note in this figure that the 0.06 and 0.08 ozone isopleths almost touch.

To rectify this situation, the user can increase the second stage tension factor on the ACCURACY card. This causes partial straightening of the curve between the points used to draw the isopleths. For example, a second run was done (with the ALREADY option to save computing time) using a tension factor of 10.0 (see Figure 5-5). Note that the isopleths are now more evenly spaced in Figure 5-5 than in Figure 5-4. The input deck for the run with the default tension factor was:

```
EMIS      8.0       0.22      0.22      0.21      0.22      0.22
0.22      0.23      0.25
PLOT
ISOP                         12.0       1.0
0.06      0.08      0.12      0.16      0.20      0.24      0.28
0.30      0.32      0.34      0.36      0.40
blank card
```

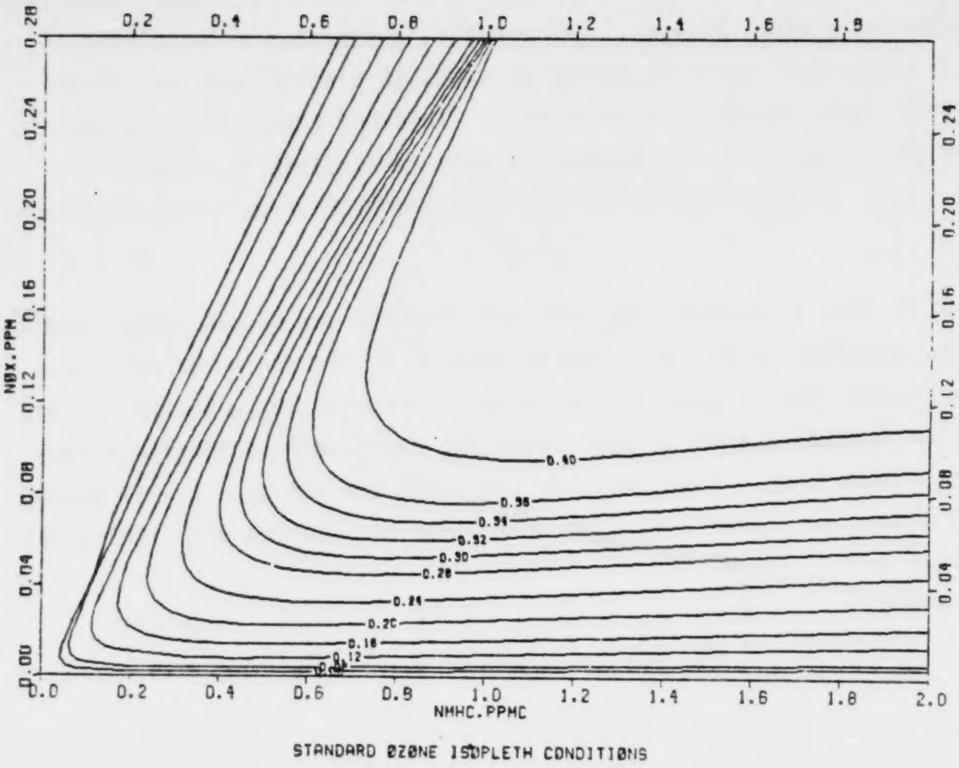

FIGURE 5-4. Isopleth Diagram with Default Tension Factor Showing Touching Isopleths

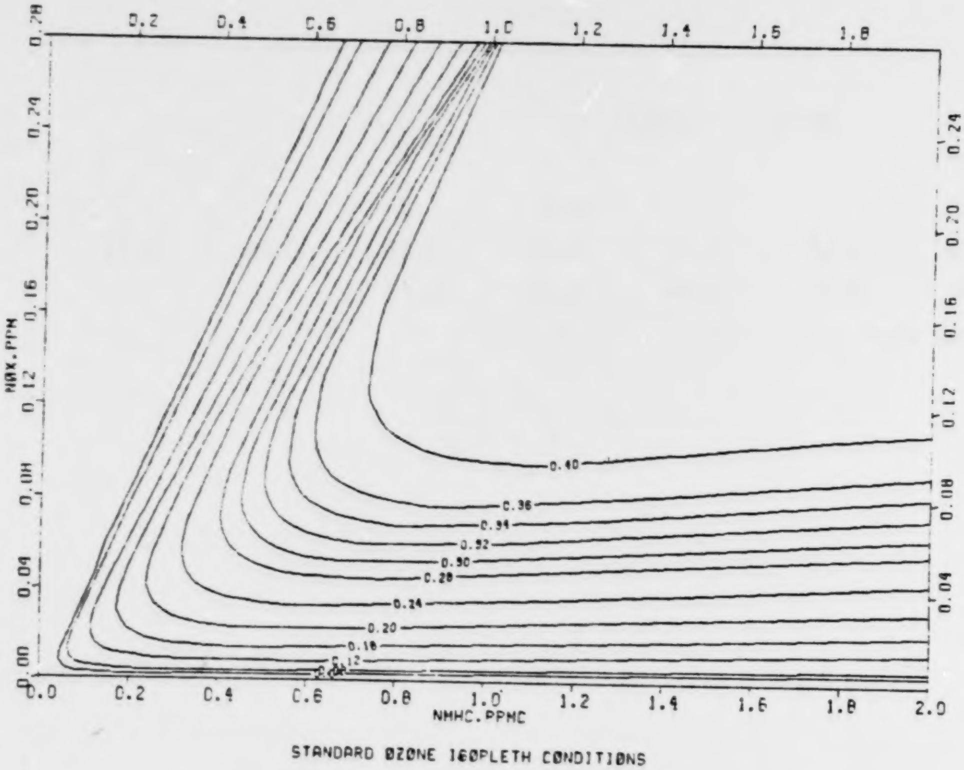

FIGURE 5-5. Isopleth Diagram with Increased Tension Factor To Eliminate Touching Isopleths

The input deck for the run with the tension factor of 10.0 was:

```
EMIS      8.0       0.22      0.22      0.21      0.22      0.22
0.22      0.23      0.25
ACCU                                                       10.0
ALRE     61.0
0.        0.        0.
 .
 .
 .
2.0        .00635    .07837
PLOT
ISOP                         12.0      1.0
0.06      0.08      0.12      0.16      0.20      0.24      0.28
0.30      0.32      0.34      0.36      0.40
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```

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## APPENDIX A

## KINETIC MECHANISM USED IN OZIPP

| Number | Reaction | Rate Constant* |
|---|---|---|
| 1 | $NO_2 + h\nu \rightarrow NO + O(^3P)$ | $k_{vary}$ |
| 2 | $O(^3P) + O_2 + M \rightarrow O_3 + M$ | $2.0 \times 10^{-5}$ $ppm^{-2}min^{-1}$ |
| 3 | $O_3 + NO \rightarrow NO_2 + O_2$ | 25.0 |
| 4 | $NO_2 + O_3 \rightarrow NO_3 + O_2$ | 0.045 |
| 5 | $NO_2 + O(^3P) \rightarrow NO + O_2$ | $1.3 \times 10^4$ |
| 6 | $NO_3 + NO \rightarrow 2NO_2$ | $1.3 \times 10^4$ |
| 7 | $NO_2 + NO_3 \rightarrow N_2O_5$ | $5.6 \times 10^3$ |
| 8 | $N_2O_5 \rightarrow NO_2 + NO_3$ | $22.0\ min^{-1}$ |
| 9 | $N_2O_5 + H_2O \rightarrow 2HNO_3$ | $2.5 \times 10^{-6}$ |
| 10 | $NO + NO_2 + H_2O \rightarrow 2HONO$ | $1.0 \times 10^{-9}$ $ppm^{-2}min^{-1}$ |
| 11 | $2HONO \rightarrow NO + NO_2 + H_2O$ | $1.0 \times 10^{-3}$ |
| 12 | $HONO + h\nu \rightarrow OH + NO$ | $k_{vary}$ |
| 13 | $OH + NO_2 \xrightarrow{M} HNO_3$ | $8.0 \times 10^3$ |
| 14 | $OH + NO \xrightarrow{M} HONO$ | $3.0 \times 10^3$ |
| 15 | $HO_2 + NO \rightarrow NO_2 + OH$ | $1.2 \times 10^3$ |
| 16 | $HO_2 + HO_2 \rightarrow HOOH + O_2$ | $8.4 \times 10^3$ |
| 17 | $HOOH + h\nu \rightarrow 2OH$ | $k_{vary}$ |
| 18 | $O_3 + h\nu \rightarrow O(^1D)$ | $k_{vary}$ |
| 19 | $O_3 + h\nu \rightarrow O(^3P)$ | $k_{vary}$ |
| 20 | $O(^1D) + M \rightarrow O(^3P) + M$ | $8.7 \times 10^4$ |
| 21 | $O(^1D) + H_2O \rightarrow 2OH$ | $5.1 \times 10^5$ |

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| Number | Reaction | Rate Constant* |
|---|---|---|
| 22 | $OH + O_3 \rightarrow HO_2 + O_2$ | 84.0 |
| 23 | $O_3 + HO_2 \rightarrow OH + 2O_2$ | 2.4 |
| 24 | $PROP + OH \rightarrow ADD$ | $2.5 \times 10^4$ |
| 25 | $ADD + NO \rightarrow X + NO_2$ | $1.0 \times 10^3$ |
| 26 | $ADD + ADD \rightarrow 2X$ | $1.2 \times 10^4$ |
| 27 | $ADD + MeO_2 \rightarrow X + MeO$ | $1.0 \times 10^3$ |
| 28 | $ADD + C_2O_2 \rightarrow X + C_2O$ | $1.0 \times 10^3$ |
| 29 | $ADD + C_3O_2 \rightarrow X + C_3O$ | $1.0 \times 10^3$ |
| 30 | $X \rightarrow HCHO + ALD2 + HO_2$ | $1.0 \times 10^5$ $min^{-1}$ |
| 31 | $PROP + O_3 \rightarrow OH + HO_2 + ALD2$ | $8.0 \times 10^{-3}$ |
| 32 | $PROP + O_3 \rightarrow OH + C_2O_3 + HCHO$ | $8.0 \times 10^{-3}$ |
| 33 | $BUT + OH \rightarrow ScO_2$ | $1.8 \times 10^3$ |
| 34 | $BUT + OH \rightarrow C_4O_2$ | $1.8 \times 10^3$ |
| 35 | $NO + C_4O_2 \rightarrow NO_2 + C_4O$ | $1.8 \times 10^3$ |
| 36 | $NO + ScO_2 \rightarrow NO_2 + ScO$ | $1.8 \times 10^3$ |
| 37 | $NO + C_3O_2 \rightarrow NO_2 + C_3O$ | $1.8 \times 10^3$ |
| 38 | $NO + C_2O_2 \rightarrow NO_2 + C_2O$ | $1.8 \times 10^3$ |
| 39 | $NO + MeO_2 \rightarrow NO_2 + MeO$ | $1.8 \times 10^3$ |
| 40 | $C_4O \rightarrow HCHO + C_3O_2$ | $7.5 \times 10^4$ $min^{-1}$ |
| 41 | $ScO \rightarrow ALD2 + C_2O_2$ | $1.0 \times 10^5$ $min^{-1}$ |
| 42 | $C_3O \rightarrow HCHO + C_2O_2$ | $8.0 \times 10^3$ $min^{-1}$ |
| 43 | $C_2O \rightarrow HCHO + MeO_2$ | $4.0 \times 10^3$ $min^{-1}$ |
| 44 | $C_4O + O_2 \rightarrow ALD4 + HO_2$ | 0.7 |
| 45 | $ScO + O_2 \rightarrow MEK + HO_2$ | 1.4 |

| Number | Reaction | Rate Constant* |
|---|---|---|
| 46 | $C_3O + O_2 \rightarrow ALD3 + HO_2$ | 0.5 |
| 47 | $C_2O + O_2 \rightarrow ALD2 + HO_2$ | 0.4 |
| 48 | $MeO + O_2 \rightarrow HCHO + HO_2$ | 0.4 |
| 49 | $HCHO + h\nu \rightarrow$ Stable Products | $k_{vary}$ |
| 50 | $HCHO + h\nu \rightarrow 2HO_2$ | $k_{vary}$ |
| 51 | $HCHO + OH \rightarrow HO_2$ | $1.5 \times 10^4$ |
| 52 | $ALD2 + h\nu \rightarrow$ Stable Products | $4.2 \times 10^{-6}$ min$^{-1}$ |
| 53 | $ALD2 + h\nu \rightarrow MeO_2 + HO_2$ | $k_{vary}$ |
| 54 | $ALD2 + OH \rightarrow C_2O_3$ | $1.5 \times 10^4$ |
| 55 | $ALD3 + h\nu \rightarrow$ Stable Products | $6.0 \times 10^{-5}$ min$^{-1}$ |
| 56 | $ALD3 + h\nu \rightarrow C_2O_2 + HO_2$ | $2.5 \times 10^{-3}$ min$^{-1}$ |
| 57 | $ALD3 + OH \rightarrow C_3O_3$ | $4.5 \times 10^4$ |
| 58 | $ALD4 + h\nu \rightarrow$ Stable Products | $6.0 \times 10^{-5}$ min$^{-1}$ |
| 59 | $ALD4 + h\nu \rightarrow C_3O_2 + HO_2$ | $1.9 \times 10^{-3}$ min$^{-1}$ |
| 60 | $ALD4 + OH \rightarrow C_4O_3$ | $4.5 \times 10^4$ |
| 61 | $ADD + C_4O_2 \rightarrow X + C_4O$ | $1.0 \times 10^3$ |
| 62 | $ADD + ScO_2 \rightarrow X + ScO$ | $1.0 \times 10^3$ |
| 63 | $C_4O_3 + NO \rightarrow C_3O_2 + NO_2$ | $8.0 \times 10^2$ |
| 64 | $C_3O_3 + NO \rightarrow C_2O_3 + NO_2$ | $8.0 \times 10^2$ |
| 65 | $C_2O_3 + NO \rightarrow MeO_2 + NO_2$ | $8.0 \times 10^2$ |
| 66 | $C_4O_3 + NO_2 \rightarrow PAN$ | $1.0 \times 10^2$ |
| 67 | $C_3O_3 + NO_2 \rightarrow PAN$ | $1.0 \times 10^2$ |
| 68 | $C_2O_3 + NO_2 \rightarrow PAN$ | $1.0 \times 10^2$ |

| Number | Reaction | Rate Constant* |
|---|---|---|
| 69 | $C_4O_2 + HO_2 \rightarrow$ Stable Products | 4.0 X $10^3$ |
| 70 | $C_3O_2 + HO_2 \rightarrow$ Stable Products | 4.0 X $10^3$ |
| 71 | $ScO_2 + HO_2 \rightarrow$ Stable Products | 4.0 X $10^3$ |
| 72 | $C_2O_2 + HO_2 \rightarrow$ Stable Products | 4.0 X $10^3$ |
| 73 | $MeO_2 + HO_2 \rightarrow$ Stable Products | 4.0 X $10^3$ |
| 74 | $C_4O_3 + HO_2 \rightarrow$ Stable Products | 4.0 X $10^3$ |
| 75 | $C_3O_3 + HO_2 \rightarrow$ Stable Products | 4.0 X $10^3$ |
| 76 | $C_2O_3 + HO_2 \rightarrow$ Stable Products | 4.0 X $10^3$ |

* Units of $ppm^{-1}min^{-1}$ unless otherwise indicated

Source: Dodge (1977).

| Symbol | Definition |
|---|---|
| $k_{vary}$ | Diurnal 1-hour average photolytic rate constant |
| PROP | $C_3H_6$ |
| BUT | $n\text{-}C_4H_{10}$ |
| ADD | $CH_3CH(OH)CH_2OO$ |
| X | $CH_3CH(OH)CH_2O$ |
| $MeO_2$ | $CH_3O_2$ |
| $C_2O_2$ | $CH_3CH_2O_2$ |
| $C_3O_2$ | $CH_3CH_2CH_2O_2$ |
| $C_4O_2$ | $CH_3CH_2CH_2CH_2O_2$ |
| $ScO_2$ | $CH_3CH(O_2)CH_2CH_3$ |
| ALD2 | $CH_3CHO$ |
| ALD3 | $CH_3CH_2CHO$ |

| Symbol | Definition |
|---|---|
| ALD4 | $CH_3CH_2CH_2CHO$ |
| $C_2O_3$ | $CH_3CO_3$ |
| $C_3O_3$ | $CH_3CH_2CO_3$ |
| $C_4O_3$ | $CH_3CH_2CH_2CO_3$ |

# APPENDIX B

## PROGRAM SOURCE LISTINGS

| Routine in OZIPP | | Page Number |
|---|---|---|
| Program | MAIN | 102 |
| Subroutine | PHOT | 108 |
| " | RATE | 110 |
| " | SOLAR | 111 |
| " | SPLNA | 113 |
| " | SPLNB | 115 |
| Function | CLOCK | 116 |
| Subroutine | RLINE | 117 |
| " | SIM | 124 |
| " | DRIVES | 127 |
| " | STIFFS | 130 |
| " | DIFFUN | 135 |
| " | OZMX | 137 |
| " | COSET | 138 |
| " | NSCORA | 139 |
| " | NSNFAC | 140 |
| " | NSBSLV | 142 |
| " | YSMER | 143 |
| " | INTERP | 144 |
| " | LINER | 145 |
| " | CURVE | 150 |
| " | ISOPLT | 153 |
| " | CURV1 | 156 |
| Function | CURV2 | 159 |
| Subroutine | KURV1 | 161 |
| " | KURV2 | 165 |
| " | FRAME | 167 |
| " | AXES | 169 |
| Block Data | SUN | 172 |
| " | MECH | 175 |
| " | GEAR | 176 |
| Function | CIRC | 177 |
| Subroutine | EMISS | 178 |
| " | CONVT | 182 |
| " | EDGMX | 183 |
| " | DEC | 184 |
| " | SOL | 185 |
| " | VVLBLF | 186 |
| " | NEWLIN | 189 |

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```
      COMMON /CALC/ NR,KR(77,5),A(77),S(77),R(77),ITYPE(77),IA(34),JA(21
     10),DILUT,TEMP,ERR,START,STOPP,SPECIS(34),TPRNT,TSTEP
      COMMON /CNTRL/ SIG,SIGMA,INFO,NPTO,XNF,RCTY,ALDX,OZIN,OZAL,HCIN,HC
     1AL,XNIN,XNAL,TSRT,DTIM,Z1,Z2,DCON,EHC,EXN,FLST,TLST
      COMMON /EMIS/ NEM,EM(11),EMHC(11),EMNOX(11),ESTRT(2),ESTOP,ESLP,EH
     1SLP,ENSLP,EC(38),ECHC(38),ECXN(38)
      COMMON /INOUT/ IN,IOUT,ITAPE
      COMMON /TITL/ ITTL(18)
      COMMON /PLTVEC/ HCT(20),OT(20),NT,OHC,HCG,PLTGRD,OXN,XNG,HC1,XN1,T
     1ICZ,DIGZ,CHRZ
      COMMON /VVLBL/ FCTR,DIST,CHRSIZ,NNCHR,OZBL
      COMMON /NEED/ HC,XN,NL,NRTO,RTO(20),OZP(20),OZN(8,20),RHO(8,20),MR
     1,OC(4),OS(2),HCS,XNS,LS,HCLL(8)
      COMMON /HOUR/ OZM,NGO,TM
      COMMON /SUNLIT/ XJ(47,10),SIGMO(31,10),PHI(31,10),Z(10),RTCON(10),
     1LAM1,INC,SLA,SLO,TZ,IY,IM,ID,ISTRT,ISTOP,IINC,IEND,SPECIE,MAXZ,ITI
     2ME(15),XZ(15),K(15),JSTRT,JSTOP,SPEC(11),MNLM(11),MXLM(11),MAXL,MA
     3XJ
      DIMENSION F(21), X(6), PLACE(6)
      DIMENSION NRTC(76), XRTC(76)
      DATA ISPD/4HISOP/,ICAL/4HCALC/,IACR/4HACCU/,IDIL/4HDILU/,IPLC/4HPL
     1AC/,IEMS/4HEMIS/,IRDY/4HALRE/,IBLK/4H    /,IPLT/4HPLOT/,ITRN/4HTRA
     2N/,ITIT/4HTITL/,IRCT/4HREAC/
C  SET DEFAULTS
      DATA HC/2.0/,XN/0.28/,NL/11/,NC/11/,MR/5/
      DATA ITTL/4HSTAN,4HDARD,4H OZO,4HNE I,4HSOPL,4HETH ,4HCOND,4HITIO,
     14HNS ,9*4H    /
      DATA IOUT/6/,KALCMP/0/,INFO/0/,NPTO/0/,KS/1/,NGO/1/
      DATA OZP/.08,.12,.16,.20,.24,.28,.30,.32,.34,.36,.40,9*0./
      DATA TSRT/0.0/,DTIM/420./,Z1/510./,Z2/630./,DCON/0.0/
      DATA DSTRT/800./,DEND/1500./,PLTGRD/0./,OHC/0./,FCTR/0.6/,OXN/0./
      DATA CHRSIZ/0.07/,TICZ/0.07/,DIGZ/0.10/,CHRZ/0.10/,HC1/8.5/,XN1/5.
     195/
      DATA SIG/1./,SIGMA/1./,RCTY/.25/,XNF/.25/,ALDX/.05/
      DATA OZIN/0./,OZAL/0./,HCIN/0./,HCAL/0./,XNIN/0./,XNAL/0./
      DATA ERR/0.01/,TEMP/303.0/,KSS/0/,KS1/0/,JS/0/
      DATA F(21)/0.0/,ESTOP/0.0/,STOPP/600./,TPRNT/60./,TSTEP/60./
      DATA PLACE/4H LOS,4H ANG,4HELES,4H, CA,4HLIF.,4H    /
      DATA SLA/34.058/,SLO/118.250/,TZ/8.0/,IY/1975/,IM/6/,ID/21/
      DATA IEM/0/,EMHC(1)/-3./,EMNOX(1)/-3./,NEM/0/
      CALL PHOT (PLACE)
C
C OPTIONS LOOP
C
    5 READ 120, IOPT,(X(I),I=1,6)
      IF (IOPT.NE.ISPD) GO TO 10
      IF (ABS(X(1)).NE.0.) HC=X(1)
      IF (ABS(X(2)).NE.0.) XN=X(2)
      IF (ABS(X(4)).NE.0.) INFO=-1
      IF (ABS(X(3)).NE.0.) NL=IFIX(X(3)+0.1)
      IF (ABS(X(3)).NE.0.) READ 130, (OZP(I),I=1,NL)
      WRITE (IOUT,145) (ITTL(I),I=1,18)
      KSTOP=JSTOP-100
      WRITE (IOUT,170) PLACE,SLA,SLO,TZ,IM,ID,IY,JSTRT,KSTOP
      NOON=SPECIE
      IF (INFO.EQ.-1) WRITE (IOUT,175) NOON
      DDTRT=DSTRT
      DDEND=DEND
      WRITE (IOUT,180) Z1,Z2,DDTRT,DDEND
      WRITE (IOUT,185) RCTY,XNF,ALDX
      IF (OZIN+HCIN+XNIN.GT.0..OR.OZAL+HCAL+XNAL.GT.0.) WRITE (IOUT,225)
      IF (OZIN+HCIN+XNIN.GT.0.) WRITE (IOUT,190) OZIN,HCIN,XNIN
      IF (OZAL+HCAL+XNAL.GT.0.) WRITE (IOUT,195) OZAL,HCAL,XNAL
      IF (NEM.GT.0) WRITE (IOUT,200) (I,I=1,NEND)
      IF (NEM.GT.0) WRITE (IOUT,205) (EM(I),I=1,NEND)
      IF (NEM.LE.-1.AND.EMHC(1).GE.-0.) WRITE (IOUT,210) (I,I=1,IEND)
      IF (NEM.LE.-1.AND.EMHC(1).GE.-0.0) WRITE (IOUT,215) (EMHC(I),I=1,I
     1END
      IF (NEM.LE.-1.AND.EMNOX(1).GE.-0.) WRITE (IOUT,220) (I,I=1,IEND)
      IF (NEM.LE.-1.AND.EMNOX(1).GE.-0.) WRITE (IOUT,215) (EMNOX(I),I=1,
     1IEND)
      CALL RLINE (NC,F,KS1,JS)
      CALL LINER (SIG,KALCMP,F)
      INFO=0
      GO TO 5
   10 IF (IOPT.NE.ICAL) GO TO 15
      NPTO=1
      WRITE (IOUT,145) (ITTL(I),I=1,18)
      KSTOP=JSTOP-100
      WRITE (IOUT,170) PLACE,SLA,SLO,TZ,IM,ID,IY,JSTRT,KSTOP
      NOON=SPECIE
      WRITE (IOUT,175) NOON
      DDTRT=DSTRT
      DDEND=DEND
      WRITE (IOUT,180) Z1,Z2,DDTRT,DDEND
      WRITE (IOUT,185) RCTY,XNF,ALDX
      IF (OZIN+HCIN+XNIN.GT.0..OR.OZAL+HCAL+XNAL.GT.0.) WRITE (IOUT,225)
      IF (OZIN+HCIN+XNIN.GT.0.) WRITE (IOUT,190) OZIN,HCIN,XNIN
      IF (OZAL+HCAL+XNAL.GT.0.) WRITE (IOUT,195) OZAL,HCAL,XNAL
      IF (NEM.GT.0) WRITE (IOUT,200) (I,I=1,NEND)
      IF (NEM.GT.0) WRITE (IOUT,205) (EM(I),I=1,NEND)
      IF (NEM.LE.-1.AND.EMHC(1).GE.-0.) WRITE (IOUT,210) (I,I=1,IEND)
      IF (NEM.LE.-1.AND.EMHC(1).GE.-0.0) WRITE (IOUT,215) (EMHC(I),I=1,I
     1END
      IF (NEM.LE.-1.AND.EMNOX(1).GE.-0.) WRITE (IOUT,220) (I,I=1,IEND)
      IF (NEM.LE.-1.AND.EMNOX(1).GE.-0.) WRITE (IOUT,215) (EMNOX(I),I=1,
     1IEND)
      IF (ABS(X(3)).NE.0.) INFO=1
      TPRNT=60.
      TSTEP=60.
      IF (ABS(X(4)).NE.0.) TPRNT=X(4)
      IF (ABS(X(5)).NE.0.) TSTEP=X(5)
      CALL SIM (X(1),X(2),ZN,1)
      IF (TM.GT.0.) WRITE (IOUT,140) ZN,TM
      IF (TM.LE.0.) WRITE (IOUT,165) ZN
      CALL LINPRT (X(1),X(2))
      NPTO=0
      INFO=0
      GO TO 5
   15 IF (IOPT.NE.IACR) GO TO 20
      IF (ABS(X(1)).NE.0.) NC=IFIX(X(1)+0.1)
      IF ((NC/2).EQ.((NC+1)/2)) NC=NC+1
      IF (ABS(X(2)).NE.0.) MR=IFIX(X(2)+0.1)
      IF (ABS(X(3)).NE.0.) ERR=X(3)
      IF (ABS(X(4)).NE.0.) SIG=X(4)
      IF (ABS(X(5)).NE.0   SIGMA=X(5)
      IF (ABS(X(6)).NE.0.) NCO=0
      GO TO 5
   20 IF (IOPT.NE.IPLC) GO TO 25
      IF (ABS(X(1)).NE.0.) SLA=X(1)
      IF (ABS(X(2)).NE.0.) SLO=X(2)
      IF (ABS(X(3)).NE.0.) TZ=X(3)
      IF (ABS(X(4)).NE.0.) IY=IFIX(X(4)+0.01)
      IF (ABS(X(5)).NE.0.) IM=IFIX(X(5)+0.01)
      IF (ABS(X(6)).NE.0.) ID=IFIX(X(6)+0.01)
      IF (ABS(X(1)).NE.0..OR.ABS(X(2)).NE.0.) READ 160, (PLACE(I),I=1,6)
      CALL PHOT (PLACE)
      GO TO 5
   25 IF (IOPT.NE.IDIL) GO TO 30
      IF (ABS(X(1)).NE.0.) Z1=X(1)
      IF (ABS(X(2)).NE.0.) Z2=X(2)
      IF (ABS(X(3)).NE.0.) DSTRT=X(3)
      IF (ABS(X(4)).NE.0.) DEND=X(4)
      JMIN=IFIX(DSTRT)-((IFIX(DSTRT)/100)*100)
      TMIN1=FLOAT((IFIX(DSTRT)/100)*60+JMIN)
      JMIN=IFIX(DEND)-((IFIX(DEND)/100)*100)
      TMIN2=FLOAT((IFIX(DEND)/100)*60+JMIN)
      DTIM=TMIN2-TMIN1
      TSRT=TMIN1-480.
      GO TO 5
   30 IF (IOPT.NE.IEMS) GO TO 55
      NEM=IFIX(X(1)+0.1)
      IEM=IFIX(ABS(X(1))+0.1)
      IF (X(1).LT.-0.999999999) GO TO 40
      DO 35 I=1,5
   35 EM(I)=ABS(X(I+1))
      IF (NEM-5.GT.0) READ 130, (EM(I),I=6,NEM)
      CALL EMISS (NEM,EM,ESTRT(1),ESTOP,ESLP,EC)
      EMHC(1)=-3.
      EMNOX(1)=-3.
      GO TO 5
   40 DO 45 I=1,5
   45 EMHC(I)=X(I+1)
      IF (EMHC(1).LT.-0.0001) GO TO 50
      IF (IEM-5.GT.0) READ 130, (EMHC(I),I=6,IEM)
      CALL EMISS (IEM,EMHC,ESTRT(1),ESTOP,EHSLP,ECHC)
   50 READ 130, (EMNOX(I),I=1,7)
      IF (EMNOX(1).LT.-0.0001) GO TO 5
      IF (IEM-7.GT.0) READ 130, (EMNOX(I),I=8,IEM)
      CALL EMISS (IEM,EMNOX,ESTRT(2),ESTOP,ENSLP,ECXN)
      GO TO 5
   55 IF (IOPT.NE.IPLT) GO TO 60
      KALCMP=1
      FCTR=0.6
      HC1=8.5
      XN1=5.95
      CHRZ=0.10
      CHRSIZ=0.07
      IF (ABS(X(1)).NE.0.) FCTR=X(1)
      PLTGRD=X(2)
      IF (ABS(X(3)).NE.0.) HC1=X(3)
      IF (ABS(X(4)).NE.0.) XN1=X(4)
      IF (ABS(X(5)).NE.0.) CHRZ=X(5)
      IF (ABS(X(6)).NE.0.) CHRSIZ=X(6)
      DICZ=CHRZ
      TICZ=CHRSIZ
      GO TO 5
   60 IF (IOPT.NE.IRCT) GO TO 65
      IF (ABS(X(1)).NE.0.) RCTY=X(1)
      IF (ABS(X(2)).NE.0.) XNF=X(2)
      IF (ABS(X(3)).NE.0.) ALDX=X(3)
      GO TO 5
   65 IF (IOPT.NE.ITIT) GO TO 70
      READ 125, (ITTL(I),I=1,18)
      GO TO 5
   70 IF (IOPT.NE.ITRN) GO TO 75
      OZIN=X(1)
      OZAL=X(2)
      HCIN=X(3)
      HCAL=X(4)
      XNIN=X(5)
      XNAL=X(6)
      GO TO 5
   75 IF (IOPT.NE.IRDY) GO TO 115
      KS1=IFIX(X(1)+0.1)
      KK=0
      JS=1
      IF (KK.EQ.KS1) GO TO 5
      WRITE (IOUT,150)
      DO 80 I=1,4
      READ 130, HCC,XNN,OC(I)
      IF (XNN.NE.0.0) RTO1=HCC/XNN
      IF (XNN.EQ.0.0) RTO1=0.00000
      WRITE (IOUT,155) HCC,XNN,RTO1,OC(I)
      KK=KK+1
      IF (I.EQ.2) HCLL(MR)=XNN
      IF (I.NE.3) GO TO 80
      RTO(1)=RTO1
      F(1)=SQRT(RTO1*RTO1+1.)
      RHO(MR,1)=F(1)*XNN
      OZN(MR,1)=OC(3)
      HCE=0.98*HCC
      NCE=1
   80 IF (KK.EQ.KS1) GO TO 5
      IF (NC.EQ.1) GO TO 95
   85 DO 90 I=1,2
      HCS=HCC
      READ 130, HCC,XNS,OS(I)
      RTO2=HCC/XNS
      WRITE (IOUT,155) HCC,XNS,RTO2,OS(I)
      KK=KK+1
      IF (KK.EQ.5) HCG=HCC
      IF (KK.EQ.5) OHC=OS(I)
      IF (KK.EQ.6) XNG=XNS
      IF (KK.EQ.6) OXN=OS(I)
   90 IF (KK.EQ.KS1) GO TO 5
   95 JK=MR-1
```

```
      NCR=(NC+1)/2
      DO 110 I=1,NC
      IF (JK+I.EQ.1) GO TO 110
  100 READ 130, HCC,XNN,ZN
      IF (HCC.GT.HCE) NCE=NCE+1
      IF (JK.EQ.MR) RTO(I)=HCC/XNN
      IF (JK.EQ.MR) F(I)=SQRT(RTO(I)*RTO(I)+1.)
      WRITE (IOUT,155) HCC,XNN,RTO(I),ZN
      IF (JK.LT.MR) GO TO 105
      IF (RTO(I).GT.1.02*RTO2.OR.RTO(I).LT.0.98*RTO2) GO TO 105
      RHO(MR,I)=SQRT(HCE*HCE*1.041232+XNS*XNS)
      OZN(MR,I)=OS(2)
      JK=MR-1
      NCE=NCE+1
      JS=JS+1
  105 OZN(JK,I)=ZN
      RHO(JK,I)=SQRT(HCC*HCC+XNN*XNN)
      IF (HCC.LE.0..AND.I.EQ.NCR) HCLL(JK)=XNN
      KK=KK+1
      IF (KK.EQ.KS1) GO TO 5
      JK=JK-1
      IF (JK.GT.0) GO TO 100
      IF (NCE.EQ.(NC+1)/2) GO TO 85
  110 JK=MR
      GO TO 85
  115 IF (IOPT.NE.IBLK) WRITE (IOUT,135) IOPT
      IF (IOPT.EQ.IBLK) STOP
      GO TO 5
C
C
  120 FORMAT (A4,6X,6F10.2)
  125 FORMAT (18A4)
  130 FORMAT (7F10.5)
  135 FORMAT (1H1,24HTHE OPTIONS INSTRUCTION ,A4,21H CANNOT BE PROCESSED
     1.)
  140 FORMAT (1H0,30X,28HMAXIMUM ONE HOUR AVE OZONE =,F7.5,12H CENTERED
     1AT,F5.0,9H MINUTES.)
  145 FORMAT (1H1,//,40X,18A4)
  150 FORMAT (1H1,//,14X,36HTHE FOLLOWING RESULTS WERE READ IN. ////1H ,
     116X,2HHC,18X,3HNOX,15X,5HRATIO,16X,5HOZONE)
  155 FORMAT (1H0,4F20.5)
  160 FORMAT (6A4)
  165 FORMAT (1H0,30X,56HMAXIMUM OZONE NOT REACHED, THE LAST ONE HOUR AV
     1ERAGE WAS,F7.5,5H PPM.)
  170 FORMAT (1H0,//,40X,40HPHOTOLYTIC RATE CONSTANTS CALCULATED FOR,///
     1,49X,6A4,///,40X,9HLATITUDE ,F10.3,//,40X,10HLONGITUDE ,F10.3,//,4
     20X,9HTIME ZONE,F7.1,//,40X,5HDATE ,5X,3(I4,3X),//,40X,5HTIME ,7X,I
     34,3X,2HTO,3X,I4,5X,19HLOCAL DAYLIGHT TIME)
  175 FORMAT (1H0,39X,10HSOLAR NOON,I7)
  180 FORMAT (1H0,//,40X,39HDILUTION DETERMINED FROM THE FOLLOWING ,//,4
     10X,17HINVERSION HEIGHTS,5X,7HINITIAL,F7.0,5X,5HFINAL,4X,F7.0,//,40
     2X,7HTIMING ,15X,5HSTART,F9.0,5X,4HSTOP,4X,F8.0)
  185 FORMAT (1H0,//,40X,26HINITIAL PROPYLENE FRACTION,F9.3,6X,7HNO2/NOX
     1,F8.3,//,40X,25HINITIAL ALDEHYDE FRACTION,F10.3)
  190 FORMAT (/,40X,13HSURFACE LAYER ,9X,5HOZONE,F8.3,6X,11HHYDROCARBON
     1,F7.3,4X,3HNOX,F7.3,4H PPM)
  195 FORMAT (/,40X,5HALOFT,17X,5HOZONE,F8.3,6X,11HHYDROCARBON,F7.3,4X,
     13HNOX,F7.3,4H PPM)                                               A   283
200  FORMAT (1H0,//,40X,50HCONTINUOUS EMISSIONS (EXPRESSED AS THE FRACT A   284
     1ION OF,//,40X,54HINITIAL NON-BACKGROUND CONCENTRATION EMITTED PER  A   285
     2HOUR),//,40X,4HHOUR,3X,10I6)                                      A   286
205  FORMAT (1H0,39X,8HFRACTION,10F6.3)                                 A   287
210  FORMAT (1H0,//,40X,58HCONTINUOUS EMISSIONS (EXPRESSED AS THE FRACT A   288
     1ON OF INITIAL,//,40X,58HNON-BACKGROUND HYDROCARBON CONCENTRATION E A   289
     2MITTED PER HOUR),//,40X,4HHOUR,3X,10I6)                           A   290
215  FORMAT (1H0,39X,8HFRACTION,10F6.3)                                 A   291
220  FORMAT (1H0,//,40X,58HCONTINUOUS EMISSIONS (EXPRESSED AS THE FRACT A   292
     1ION OF INITIAL,//,40X,50HNON-BACKGROUND NOX CONCENTRATION EMITTED  A   293
     2PER HOUR),//,40X,4HHOUR,3X,10I6)                                  A   294
225  FORMAT (1H0,//,40X,26HTRANSPORTED CONCENTRATIONS )                 A   295
     END                                                                A   296-
```

# Subroutine PHOT

```
      SUBROUTINE PHOT (PLACE)
C
C    ****     RATE CONSTANT CALCULATIONS FOR FIRST ORDER PHOTOCHEMICAL RE
C
      REAL K
      COMMON /SUNLIT/ XJ(47,10),SIGMA(31,10),PHI(31,10),Z(10),RTCON(10),
     1LAM1,INC,SLA,SLO,TZ,IY,IM,ID,ISTRT,ISTOP,IINC,IEND,SPECIE,MAXZ,ITI
     2ME(015),XZ(015),K(015),JSTRT,JSTOP,SPEC(11),MNLM(11),MXLM(11),MAXL
     3,MAXJ
      COMMON /PHOTON/ CF(45,8),P(15,9),IPH(9)
      DIMENSION D(2), C(27), W(45), V(5), TMS(16), PLACE(6)
      DATA D/0.0,0.0/,JSTRT/0800/,JSTOP/1900/,IINC/60/
C
      IEND=15
      NTM=IEND
      TIME=JSTRT
      DO 5 II=1,IEND
C
C    ****     CALL SUBROUTINE TO COMPUTE ZENITH ANGLES FROM TIME OF DAY
C
      XC=0.0
      TSTD=TIME-100.
      IF (TSTD.LT.0.) TSTD=TSTD+2400.
      CALL SOLAR (SLA,SLO,TZ,IY,IM,ID,TSTD,XC,5)
      ITIME(II)=TIME
      XZ(II)=90.-XC
      TIME=CLOCK(TIME,IINC)
    5 CONTINUE
C
      DO 20 L=1,MAXL
      SPECIE=SPEC(L)
      ISTRT=(MNLM(L)-LAM1)/INC+1
      ISTOP=(MXLM(L)-LAM1)/INC+1
      DO 10 M=1,MAXZ
C
C    ****     CALL SUBROUTINE TO CALCULATE RATE CONSTANTS
C
      CALL RATE (L,M,MNLM(L),MXLM(L),RTCON(M))
   10 CONTINUE
C
C    ****     CALL FIRST SUBROUTINE FOR SPLINE INTERPOLATION OF RATE CONS
C
      CALL SPLNA (MAXZ,Z,RTCON,2,D,C,W)
      DO 15 II=1,IEND
      V(1)=XZ(II)
      P(II,L)=0.
      K(II)=P(II,L)
      IF (V(1).GT.90.0) GO TO 15
C
C    ****     CALL SECOND SUBROUTINE IN SPLINE INTERPOLATION SCHEME
C
      CALL SPLNB (MAXZ,Z,RTCON,C,V)
      P(II,L)=AMAX1(0.0,V(2))
      K(II)=P(II,L)
   15 CONTINUE
C
   20 CONTINUE
```

```
C     DETERMINE TIME OF SOLAR NOON
      DO 25 I=2,IEND
   25 IF (XZ(I).GT.XZ(I-1)) GO TO 30
      I=IEND
   30 TIME=ITIME(I-1)
      XA=XZ(I-1)
      DO 35 I=1,60
      SPECIE=TIME
      TIME=CLOCK(TIME,1)
      TSTD=TIME-100.
      IF (TSTD.LT.0.) TSTD=TSTD+2400.
      XB=XA
      CALL SOLAR (SLA,SLO,TZ,IY,IM,ID,TSTD,XC,5)
      XA=90.-XC
   35 IF (XA.GT.XB) GO TO 40
   40 DO 45 I=1,IEND
      TMS(I)=60.*FLOAT(I-1)
   45 P(I,3)=P(I,3)+P(I,MAXL)
      DO 55 L=1,8
      DO 50 I=2,IEND
      NMM=IEND+2-I
   50 IF (P(NMM-1,L).GT.0.) GO TO 55
   55 CALL SPLNA (NMM,TMS,P(1,L),2,D,CF(1,L),W)
      RETURN
      END
```

## Subroutine RATE

```
      SUBROUTINE RATE (L,NZ,MINLAM,MAXLAM,SUM)
      REAL K
      COMMON /SUNLIT/ XJ(47,10),SIGMA(31,10),PHI(31,10),Z(10),RTCON(10),
     1LAM1,INC,SLA,SLO,TZ,IY,IM,ID,ISTRT,ISTOP,IINC,IEND,SPECIE,MAXZ,ITI
     2ME(015),XZ(015),K(015),JSTRT,JSTOP,SPEC(11),MNLM(11),MXLM(11),MAXL
     3,MAXJ
C
C     ****    THIS SUBROUTINE CALCULATES A SINGLE RATE CONSTANT ACCORDING
C     ****        THE GIVEN INPUTS
C
      SUM=0.0
      DO 5 I=MINLAM,MAXLAM,INC
       II=(I-LAM1)/INC+1
       IJ=II
       IF (L.EQ.MAXL) IJ=II-16
      SUM=SUM+XJ(II,NZ)*1.0E+15*SIGMA(IJ,L)*PHI(IJ,L)
    5 CONTINUE
      SUM=SUM*60.
      RETURN
      END
```

# Subroutine SOLAR

```
      SUBROUTINE SOLAR (SLA,SLO,TZ,IY,IM,ID,TIME,D,NV)
C***
C***     SLA...  LATITUDE (DEG)  SOUTH = MINUS
C***     SLO...  LONGITUDE (DEG)  EAST = MINUS
C***     TZ...  TIME ZONE
C***            ALSO INCLUDES FRACTION IF LOCAL TIME IS NOT
C***             STANDARD MERIDIAN TIME.  E.G. POONA, INDIA 5.5
C***     IY..  YEAR
C***     IM..  MONTH
C***     ID..  DAY
C***     TIME.. LOCAL STANDARD TIME IN HOURS AND MINUTES.
C***            1 30 PM = 1330  ** STANDARD TIME **
C***     D..  RETURNED VALUE
C***     NV..  VALUE TO BE RETURNED, SELECTED AS FOLLOWS....
C***           1...  DECLINATION (DEG.)
C***           2...  EQUATION OF TIME ADJUSTMENT (HRS.)
C***           3...  TRUE SOLAR TIME (HRS.)
C***           4...  HOUR ANGLE (DEG.)
C***           5...  SOLAR ELEVATION (DEG.)
C***           6...  OPTICAL AIRMASS
C***     0 ' NV ' 7.  OTHERWISE, D = 9999.
C***
      DIMENSION MD(11)
      DATA MD/31,29,31,30,31,30,2*31,30,31,30/
      DATA A,B,C,SIGA/0.15,3.885,1.253,279.9348/
      RAD=572957.75913E-4
      SDEC=39784.988432E-5
      RE=1.
      IF (SLO.LT.0.) RE=-1.
      KZ=TZ
      TC=(TZ-KZ)*RE
      TZZ=KZ*RE
      SLB=SLA/RAD
      K=ID
      TIMH=TIME/100.
      I=TIMH
      TIMLOC=(TIMH-I)/0.6+I+TC
      IMC='M-1
      IF (IMC.LT.1) GO TO 10
      DO 5 I=1,IMC
    5 K=K+MD(I)
   10 LEAP=1
      NL=MOD(IY,4)
      IF (NL.LT.1) LEAP=2
      SMER=TZZ*15.
      TK=((SMER-SLO)*4.)/60.
      KR=1
      IF (K.GE.61.AND.LEAP.LT.2) KR=2
      DAD=(TIMLOC+TZZ)/24.
      DAD=DAD+K-KR
      DF=DAD*360./365.242
      DE=DF/RAD
      DESIN=SIN(DE)
      DECOS=COS(DE)
      DESIN2=SIN(DE*2.)
      DECOS2=COS(DE*2.)
      SIG=SIGA+DF+1.914827*DESIN-0.079525*DECOS+0.019938*DESIN2-0.00162*
```

```
     1DECOS2
      SIG=SIG/RAD
      DECSIN=SDEC*SIN(SIG)
      EFFDEC=ASIN(DECSIN)
      IF (NV.NE.1) GO TO 15
      D=EFFDEC*RAD
      RETURN
   15 EQT=0.12357*DESIN-0.0[illegible]289*DECOS+0.153809*DESIN2+0.060783*DECOS2
      IF (NV.NE.2) GO TO 20
      D=EQT
      RETURN
   20 TST=TK+TIMLOC-EQT
      IF (NV.NE.3) GO TO 25
      D=TST
      IF (D.LT.0.) D=D+24.
      IF (D.GE.24.) D=D-24.
      RETURN
   25 HRANGL=ABS(TST-12.)*15.
      IF (NV.NE.4) GO TO 30
      D=HRANGL
      RETURN
   30 HRANGL=HRANGL/RAD
      SOLSIN=DECSIN*SIN(SLB)+COS(EFFDEC)*COS(SLB)*COS(HRANGL)
      SOLEL=ASIN(SOLSIN)*RAD
      IF (NV.NE.5) GO TO 35
      D=SOLEL
      RETURN
   35 IF (NV.NE.6) GO TO 40
      IF (SOLEL.LE.0.) GO TO 40
      TK=SOLEL+B
      E=1./TK**C
      D=1./(A*E+SOLSIN)
      RETURN
   40 D=9999.
      RETURN
      END
```

# Subroutine SPLNA

```
      SUBROUTINE SPLNA (N,X,Y,J,D,C,W)
      DIMENSION X(10), Y(10), D(2), C(30), W(30)
C     -----------------------------------------------------------------
C             OVER THE INTERVAL X(I) TO X(I+1), THE INTERPOLATING
C             POLYNOMIAL
C                  Y=Y(I)+A(I)*Z+B(I)*Z**2+E(I)*Z**3
C             WHERE Z=(X-X(I))/(X(I+1)-X(I))
C             IS USED. THE COEFFICIENTS A(I),B(I) AND E(I) ARE COMPUTED
C             BY SPLNA AND STORED IN LOCATIONS C(3*I-2),C(3*I-1) AND
C             C(3*I) RESPECTIVELY.
C             WHILE WORKING IN THE ITH INTERVAL,THE VARIABLE Q WILL
C             REPRESENT Q=X(I+1) - X(I), AND Y(I) WILL REPRESENT
C             Y(I+1)-Y(I)
C     -----------------------------------------------------------------
C
      Q=X(2)-X(1)
      YI=Y(2)-Y(1)
      IF (J.EQ.2) GO TO 5
C     -----------------------------------------------------------------
C             IF THE FIRST DERIVATIVE AT THE END POINTS IS GIVEN,
C             A(1) IS KNOWN, AND THE SECOND EQUATION BECOMES
C             MERELY B(1)+E(1)=YI - Q*D(1).
C     -----------------------------------------------------------------
      C(1)=Q*D(1)
      C(2)=1.0
      W(2)=YI-C(1)
      GO TO 10
C     -----------------------------------------------------------------
C             IF THE SECOND DERIVATIVE AT THE END POINTS IS GIVEN
C             B(1) IS KNOWN, THE SECOND EQUATION BECOMES
C             A(1)+E(1)=YI-0.5*Q*Q*D(1). DURING THE SOLUTION OF
C             THE 3N-4 EQUATIONS,A1 WILL BE KEPT IN CELL C(2)
C             INSTEAD OF C(1) TO RETAIN THE TRIDIAGONAL FORM OF THE
C             COEFFICIENT MATRIX.
C     -----------------------------------------------------------------
    5 C(2)=0.0
      W(2)=0.5*Q*Q*D(1)
   10 M=N-2
      IF (M.LE.0) GO TO 20
C     -----------------------------------------------------------------
C             UPPER TRIANGULARIZATION OF THE TRIDIAGONAL SYSTEM OF
C             EQUATIONS FOR THE COEFFICIENT MATRIX FOLLOWS--
C     -----------------------------------------------------------------
      DO 15 I=1,M
      AI=Q
      Q=X(I+2)-X(I+1)
      H=AI/Q
      C(3*I)=-H/(2.0-C(3*I-1))
      W(3*I)=(-YI-W(3*I-1))/(2.0-C(3*I-1))
      C(3*I+1)=-H*H/(H-C(3*I))
      W(3*I+1)=(YI-W(3*I))/(H-C(3*I))
      YI=Y(I+2)-Y(I+1)
      C(3*I+2)=1.0/(1.0-C(3*I+1))
   15 W(3*I+2)=(YI-W(3*I+1))/(1.0-C(3*I+1))
C     -----------------------------------------------------------------
C             E(N-1) IS DETERMINED DIRECTLY FROM THE LAST EQUATION
C             OBTAINED ABOVE, AND THE FIRST OR SECOND DERIVATIVE
```

```
C               VALUE GIVEN AT THE END POINT.
C     ----------------------------------------------------------------
   20 IF (J.EQ.1) GO TO 25
      C(3*N-3)=(Q*Q*D(2)/2.0-W(3*N-4))/(3.0-C(3*N-4))
      GO TO 30
   25 C(3*N-3)=(Q*D(2)-YI-W(3*N-4))/(2.0-C(3*N-4))
   30 M=3*N-6
      IF (M.LE.0) GO TO 40
C     ----------------------------------------------------------------
C               BACK SOLUTION FOR ALL COEFFICENTS EXCEPT
C               A(1) AND B(1) FOLLOWS--
C     ----------------------------------------------------------------
      DO 35 II=1,M
      I=M-II+3
   35 C(I)=W(I)-C(I)*C(I+1)
   40 IF (J.EQ.1) GO TO 45
C     ----------------------------------------------------------------
C               IF THE SECOND DERIVATIVE IS GIVEN AT THE END POINTS,
C               A(1) CAN NOW BE COMPUTED FROM THE KNOWN VALUES OF
C               B(1) AND E(1). THEN A(1) AND B(1) ARE PUT INTO THEIR
C               PROPER PLACES IN THE C ARRAY.
C     ----------------------------------------------------------------
      C(1)=Y(2)-Y(1)-W(2)-C(3)
      C(2)=W(2)
      RETURN
   45 C(2)=W(2)-C(3)
      RETURN
      END
```

## Subroutine SPLNB

```
      SUBROUTINE SPLNB (N,X,Y,C,V)
      DIMENSION X(10), Y(10), C(30), V(5)
      V(5)=2.0
      LIM=N-1
C                 ------------------------------------------------------
C                 DETERMINE IN WHICH INTERVAL THE INDEPENDENT
C                 VARIABLE,V(1),LIES.
C                 ------------------------------------------------------
      DO 5 I=2,LIM
    5 IF (V(1).LT.X(I)) GO TO 10
      I=N
      IF (V(1).GT.X(N)) V(5)=3.0
      GO TO 15
   10 IF (V(1).LT.X(1)) V(5)=1.0
C                 ------------------------------------------------------
C                 Q IS THE SIZE OF THE INTERVAL CONTAINING V(1).
C                 ------------------------------------------------------
C                 Z IS A LINEAR TRANSFORMATION OF THE INTERVAL
C                 ONTO (0,1) AND IS THE VARIABLE FOR WHICH
C                 THE COEFFICIENTS WERE COMPUTED BY SPLNA.
C                 ------------------------------------------------------
   15 Q=X(I)-X(I-1)
      Z=(V(1)-X(I-1))/Q
      V(2)=((Z*C(3*I-3)+C(3*I-4))*Z+C(3*I-5))*Z+Y(I-1)
      V(3)=((3.*Z*C(3*I-3)+2.0*C(3*I-4))*Z+C(3*I-5))/Q
      V(4)=(6.*Z*C(3*I-3)+2.0*C(3*I-4))/(Q*Q)
      RETURN
      END
```

## Function CLOCK

```
      FUNCTION CLOCK (T1,IINC)
C
C     ****    ADD A TIME IN MINUTES TO A 2400 HOUR TIME AND RETURN A 2400
C     ****    HOUR TIME
C
      T2=IINC
      I100=T1/100
      T3=T1-100.0*I100+T2
      I100=I100+INT(T3/60)
      CLOCK=I100*100.0+T3-60.0*INT(T3/60)
      RETURN
      END
```

## Subroutine RLINE

```
      SUBROUTINE RLINE (NC,F,KS1,JS)
      COMMON /NEED/ HC,XN,NL,NRTO,RTO(20),OZP(20),OZN(8,20),RHO(8,20),MR
     1,OC(4),OS(2),HCS,XNS,LS,HCLL(8)
      COMMON /CNTRL/ SIG,SIGMA,INFO,NPTO,XNF,RCTY,ALDX,OZIN,OZAL,HCIN,HC
     1AL,XNIN,XNAL,TSRT,DTIM,Z1,Z2,DCON,EHC,EXN,FLST,TLST
      COMMON /INOUT/ IN,IOUT,ITAPE
      COMMON /PLTVEC/ HCT(20),OT(20),NT,OHC,HCG,PLTGRD,OXN,XNG,HC1,XN1,T
     1ICZ,DIGZ,CHRZ
      DIMENSION R(20), F(21), YP(12), TMP(12), OE(20), XNE(20)
      EQUIVALENCE (NR,NRTO), (RTO,R)
      RLBK(A,B1,B2,B3)=A*(B1-B2)/(B3-B2)
      KFACT=KS1-6+JS
      IF (NC.EQ.1) KFACT=KFACT+2
      KS=MAX0(KFACT/MR,0)
      KS=MIN0(KS,NC)
      KSS=MAX0(KFACT-KS*MR,0)
      KS=KS+1
      IF (KS.GT.NC.AND.KSS.EQ.2) GO TO 5
      IF (INFO.EQ.0) WRITE (IOUT,365)
      IF (INFO.LT.0) WRITE (IOUT,370)
    5 DO 15 J=1,NL
      M=J.
      DO 10 L=J,NL
   10 IF (OZP(L).LT.OZP(M)) M=L
      IF (M.EQ.J) GO TO 15
      SV=OZP(J)
      OZP(J)=OZP(M)
      OZP(M)=SV
   15 CONTINUE
      NR=NC
      NSHC=0
      NSXN=0
      KK=0
      MR1=MR-1
      INX=1
      NCR=(NR+1)/2
      TOL=1.0-(0.17/(SQRT(FLOAT(NR))))
      KSN=KS1+1
      IF (KSN.GT.7) GO TO 40
      GO TO (20,25,30,35,40,40,40),KSN
C   DO CORNERS.
   20 CALL SIM (0.,0.,OC(1),INX)
   25 CALL SIM (0.,XN,OC(2),INX)
   30 IF (KS.EQ.1) CALL SIM (HC,XN,OZN(MR,1),INX)
      OC(3)=OZN(MR,1)
   35 CALL SIM (HC,0.,OC(4),INX)
   40 DO 45 LS=1,NL
   45 IF (OC(1).LT.OZP(LS)) GO TO 50
      WRITE (IOUT,355) OC(1)
      STOP
   50 IF (LS.GT.1) WRITE (IOUT,360) OZP(LS)
      IF (OZP(LS).GT.OC(3)) GO TO 345
      NCYC=0
C   DO DOUBLE ROLLBACK ON EDGES
      IF (KSN.GE.7) GO TO 75
      HCG=RLBK(HC,OZP(LS),OC(2),OC(3))
      XNG=RLBK(XN,OZP(LS),OC(4),OC(3))
      IF (HCG.LE.0.) HCG=HC/20.
      IF (XNG.LE.0.) XNG=XN/10.
      IF (NCR.EQ.1) GO TO 90
      GO TO (55,55,55,55,55,65,75),KSN
   55 OS(1)=OZP(LS)
      INX=-1
   60 CALL SIM (HCG,XN,OS(1),INX)
      OHC=OS(1)
      IF (INX.NE.-1) GO TO 65
      HCG1=RLBK(HCG,OZP(LS),OC(2),OS(1))
      IF (HCG1.GT.0.5*HC) HCG=HC/3.
      IF (HCG1.LE.0.5*HC) HCG=(RLBK(HC-HCG,OZP(LS),OS(1),OC(3))+HCG+HCG1
     1)/2.
      INX=1
      GO TO 60
   65 OS(2)=OZP(LS)
      INX=-1
   70 CALL SIM (HC,XNG,OS(2),INX)
      OXN=OS(2)
      IF (INX.NE.-1) GO TO 75
      XNG1=RLBK(XNG,OZP(LS),OC(4),OS(2))
      IF (XNG1.GT.0.5*XN) XNG=XN/3.
      IF (XNG1.LE.0.5*XN) XNG=(RLBK(XN-XNG,OZP(LS),OS(2),OC(3))+XNG+XNG1
     1)/2.
      INX=1
      GO TO 70
   75 IF (KS.GT.NR.AND.KSS.EQ.2) GO TO 245
      IF (KS.GT.NR.AND.KSS.EQ.1) GO TO 80
      HCS=RLBK(HC-HCG,OZP(LS),OS(1),OC(3))+HCG
      IF (HCS.LE.0.) HCS=HCG
   80 XNS=RLBK(XNG,OZP(LS),OC(4),OS(2))
      IF (XNS.GT.XNG) XNS=RLBK(XN-XNG,OZP(LS),OS(2),OC(3))+XNG
      IF (KS.GT.NR) GO TO 245
      IF (KS.GT.NCR) XSS=XNS
      IF (KS.GT.NCR) OSS=OS(2)
      IF (KS.LT.2) GO TO 90
      IF (KS.EQ.2) GO TO 85
      HTT1=RHO(MR,KS-2)*R(KS-2)/F(KS-2)
      XNN1=RHO(MR,KS-2)/F(KS-2)
   85 HTT=RHO(MR,KS-1)*R(KS-1)/F(KS-1)
      XNN=RHO(MR,KS-1)/F(KS-1)
      IF (KSS.EQ.0) GO TO 90
      HCC=RHO(MR,KS)*R(KS)/F(KS)
      XNX=RHO(MR,KS)/F(KS)
      GO TO 95
   90 XNX=XN
   95 XNX1=0.
      ICNT=KS-1
      DO 240 I=KS,NR
      ICNT=ICNT+1
      IF (I.GT.1) GO TO 100
      HTT=HC
      XNN=XN
      IF (KSS) 175,165,175
  100 IF (I-NCR-1) 105,125,130
  105 OZC=OZN(MR,I-1)*(OZP(LS)/OZN(MR,I-1))**(1./FLOAT(NCR+2-I))
      IF (KSS.NE.0) GO TO 120
      HSS=HCS
      OSS=OS(1)
      IF (OS(1).GT.OZC) HSS=0.
      IF (OS(1).GT.OZC) OSS=OC(2)
      IF (ICNT.GT.2) GO TO 110
      HCC=RLBK(HTT-HSS,OZC,OSS,OZN(MR,I-1))+HSS
      IF (OC(3).GT.OZP(NL)) JJ=NCR-1
      IF (OC(3).LE.OZP(NL)) JJ=NCR
      HCC1=HC-(HC-HCS)/FLOAT(JJ)
      HCC=AMAX1(HCC,HCC1)
      GO TO 120
  110 HCC=HTT1-RLBK(HTT1-HTT,OZC,OZN(MR,I-2),OZN(MR,I-1))
      A=RLBK(HTT-HSS,OZC,OSS,OZN(MR,I-1))+HSS
      BX=HTT-HCC
      AX=A-HCS
      IF (OC(3)-OZN(MR,2).GT.0) GO TO 115
      AX=0.
      BX=1.
  115 HCC=(HCC*AX+A*BX)/(AX+BX)
      HCC1=HTT-(HTT-HCS)/AMAX0(NCR+1-I,2)
      HCC=AMAX1(HCC,HCC1)
  120 IF (HCC.GT.TOL*HTT) HCC=TOL*HTT
      HMR4=HC-(FLOAT(I-1)*HC/FLOAT(NCR))
      IF (HCC.LT.HMR4) HCC=HMR4
      HTT1=HTT
      HTT=HCC
      XNN=XN
      IF (KSS) 175,155,175
  125 OZC=OC(3)*(OZP(LS)/OC(3))**(1./FLOAT(NCR))
      XNN=XN
      OZL=OC(3)
      OSS=OZP(LS)
      XSS=XNS
      ICNT=0
      IF (KSS) 150,140,150
  130 OZC=OZN(MR,I-1)*(OZP(LS)/OZN(MR,I-1))**(1./FLOAT(NR+2-I))
      OZL=OZN(MR,I-1)
      IF (KS.LE.NCR) GO TO 135
      ICNT=KS-NCR-1
  135 ICNT=ICNT+1
      IF (KSS.NE.0) GO TO 150
      IF (ICNT.LE.2) GO TO 140
      XNX1=XNN1-RLBK(XNN1-XNN,OZC,OZN(MR,I-2),OZN(MR,I-1))
  140 IF (XNN.GT.XSS) GO TO 145
      XSS=0.
      OSS=OC(4)
      XNS=XNS*0.5
  145 XNX=RLBK(XNN-XSS,OZC,OSS,OZL)+XSS
      IF (XNX1.GT.0.0.AND.XNX1.LT.XN) XNX=(XNX+XNX1)/2.0
      IF (OC(3).GT.OZP(NL)) L=1
      IF (OC(3).LE.OZP(NL)) L=2
      IF (NCR.GT.2) XNX=AMAX1(XNX,XNN-(XNN-XNS)/FLOAT(NR+L-I))
      IF (I.EQ.NR) XNX=(XNN+2.0*XNS)/3.0
      IF (I.EQ.NR.AND.XNX.LE.O.) XNX=XNN/2.
      IF (NCR.LE.2) XNX=XN/3.0
      IF (XNX.LT.1.1*XNG.AND.XNX.GT.0.9*XNG) XNX=XNG
  150 IF (XNX.GT.TOL*XNN) XNX=TOL*XNN
      XNN1=XNN
      XNN=XNX
      HTT=HC
      IF (KSS.NE.0) GO TO 175
  155 IF (OZN(MR,I-1).GT.1.1*OZP(LS)) GO TO 165
      IF (IABS(NCR-I).LE.2) GO TO 165
      GAP=0.
      NCOUNT=I-2
      IF (I.LE.(NR/2+1)) NSTART=1
      IF (I.GT.(NR/2+1)) NSTART=NR/2+1
      DO 160 JJ=NSTART,NCOUNT
      GAP1=OZN(MR,JJ)-OZN(MR,JJ+1)
      IF (GAP1.LT.GAP) GO TO 160
      GAP=GAP1
      HTT=((R(JJ)*RHO(MR,JJ))/F(JJ)+(R(JJ+1)*RHO(MR,JJ+1))/F(JJ+1))/2.0
      XNN=HTT/((R(JJ)+R(JJ+1))/2.)
  160 CONTINUE
  165 R(I)=HTT/XNN
      F(I)=SQRT(R(I)*R(I)+1.)
      RHO(MR,I)=XNN*F(I)
      IF (XNX.EQ.XNG) OZN(MR,I)=OS(2)
      IF (I.EQ.1.OR.XNX.EQ.XNG) GO TO 175
      IF (OZP(LS).GE.OC(2)) GO TO 170
      IF (I.NE.NCR) GO TO 170
      R(I)=0.
      F(I)=1.
      RHO(MR,I)=XN
      HTT=0.
      HCLL(MR)=XN
      XNN=XN
  170 CALL SIM (HTT,XNN,OZN(MR,I),INX)
  175 IF (KSS.EQ.0) KSS1=2
      IF (KSS.NE.0) KSS1=KSS+1
      IF (MR1) 240,240,180
  180 IF (MR.EQ.2) GO TO 200
      IF (KSS1.GT.MR1) GO TO 195
      DO 190 J=KSS1,MR1
      K=MR-J+1
      OZC=OZN(K+1,I)*(OZP(LS)/OZN(K+1,I))**(1./FLOAT(K))
      IF (K.EQ.MR1) GO TO 185
      RHO1=RHO(K+2,I)-RLBK(RHO(K+2,I)-RHO(K+1,I),OZC,OZN(K+2,I),OZN(K+1,
     1I))
  185 RHO(K,I)=RLBK(RHO(K+1,I),OZC,OC(1),OZN(K+1,I))
      IF (K.EQ.MR1) RHO1=RHO(K,I)
      IF (RHO1.GT.0.) RHO(K,I)=(RHO1+RHO(K,I))/2.0
      FK=AMAX0(K-2,2)
      RHO(K,I)=AMAX1(RHO(K,I),RHO(K+1,I)-(RHO(K+1,I)/FK))
      IF (RHO(K,I).GE.RHO(K+1,I)) RHO(K,I)=RHO(K+1,I)-(RHO(K+1,I)/FK)
      XNX=RHO(K,I)/F(I)
      HCC=R(I)*XNX
      IF (I.EQ.NCR.AND.OZP(LS).LT.OC(2)) HCLL(K)=XNX
      CALL SIM (HCC,XNX,OZN(K,I),INX)
  190 CONTINUE
  195 IF (OZN(2,I).LT.OZP(LS)) RHO(1,I)=0.9*RHO(2,I)
      IF (OZN(2,I).LT.OZP(LS)) GO TO 215
  200 OZN(1,I)=OC(1)
      SX=-SIG*3.
      IT=1
      RHO(1,I)=0.                                                       H 229
      CALL EDGMX (RHO(1,I),OZN(1,I),MR,HMX,OZHX,LX)                     H 230
      MM=LX+1                                                           H 231
  205 RHO(1,I)=0.                                                       H 232
      CALL CURV1 (MM,OZN(1,I),RHO(1,I),SP1,SP2,YP,TMP,SX)               H 233
      RHO(1,I)=CURV2(OZP(LS),MR,OZN(1,I),RHO(1,I),YP,SX,IT)             H 234
      INX=-2                                                            H 235
      IF (IT.GT.0) GO TO 210                                            H 236
      SX=SX*10.                                                         H 237
      SX=AMAX1(-50.,SX)                                                 H 238
      GO TO 205                                                         H 239
  210 IF (RHO(1,I).GT.0.9*RHO(2,I)) RHO(1,I)=0.9*RHO(2,I)               H 240
      IF (RHO(1,I).LE.0.) RHO(1,I)=.5*RHO(2,I)                          H 241
      IF (RHO(1,I).GE.RHO(2,I)) RHO(1,I)=0.5*RHO(2,I)                   H 242
  215 XNX=RHO(1,I)/F(I)                                                 H 243
      HCC=XNX*R(I)                                                      H 244
      OZN(1,I)=OZP(LS)                                                  H 245
      IF (OZP(LS).LT.OC(2).AND.I.EQ.NCR) HCLL(1)=XNX                    H 246
      CALL SIM (HCC,XNX,OZN(1,I),INX)                                   H 247
      IF (INX.NE.-2) GO TO 235                                          H 248
      IF (OZN(1,I)-OZP(LS)) 220,230,225                                 H 249
  220 RHO(1,I)=0.8*RLBK((RHO(2,I)-RHO(1,I)),OZP(LS),OZN(1,I),OZN(2,I))+R H 250
     1HO(1,I)                                                           H 251
      GO TO 230                                                         H 252
  225 RHO(1,I)=0.9*RLBK(RHO(1,I),OZP(LS),OC(1),OZN(1,I))                H 253
  230 INX=1                                                             H 254
      GO TO 215                                                         H 255
  235 KSS=0                                                             H 256
  240 CONTINUE                                                          H 257
C  CHECK FOR INCREASING RATIOS                                          H 258
  245 DO 260 I=1,NR                                                     H 259
      K=I                                                               H 260
      DO 250 J=1,NR                                                     H 261
  250 IF (R(J).LT.R(K)) K=J                                             H 262
      IF (K.EQ.I) GO TO 260                                             H 263
      SV=R(I)                                                           H 264
      R(I)=R(K)                                                         H 265
      R(K)=SV                                                           H 266
      SV=F(I)                                                           H 267
      F(I)=F(K)                                                         H 268
      F(K)=SV                                                           H 269
      DO 255 J=1,MR                                                     H 270
      SV=OZN(J,I)                                                       H 271
      OZN(J,I)=OZN(J,K)                                                 H 272
      OZN(J,K)=SV                                                       H 273
      SV=RHO(J,I)                                                       H 274
      RHO(J,I)=RHO(J,K)                                                 H 275
  255 RHO(J,K)=SV                                                       H 276
  260 CONTINUE                                                          H 277
C  DO SPECIAL CALCULATIONS                                              H 278
      KSS1=KSS+1                                                        H 279
      IF (OZP(LS).LT.OC(2)) NCR1=NCR-1                                  H 280
      IF (OZP(LS).GE.OC(2)) NCR1=NCR                                    H 281
      NN=NCR1+1                                                         H 282
      SX=-20.*SIG/FLOAT(NN)                                             H 283
      IF (NCR.NE.1) GO TO 265                                           H 284
      OT(1)=OC(2)                                                       H 285
      HCT(1)=0.
      OT(2)=OHC
      HCT(2)=HCG
      OT(3)=OC(3)
      HCT(3)=HC
      III=0
      NN=3
      GO TO 295
  265 DO 270 I=1,NCR1
      IF (OZP(LS).LT.OC(2)) L=I+1
      IF (OZP(LS).GE.OC(2)) L=I
      OT(I+2)=OZN(MR,L)
  270 HCT(I+2)=RHO(MR,L)*R(L)/F(L)
      OT(1)=OC(2)
      HCT(1)=0.
      OT(2)=OHC
      HCT(2)=HCG
      NN=NN+1
      IF (KSS1.GT.1) GO TO 300
      IT=1
  275 CALL CURV1 (NN,OT,HCT,SP1,SP2,YP,TMP,SX)
      DO 280 LK=1,NL
  280 IF (OZP(LK).GE.OC(2)) GO TO 285
      LK=NL
  285 HCS=CURV2(OZP(LK),NN,OT,HCT,YP,SX,IT)
      IF (IT.GT.0) GO TO 290
      SX=SX*10.
      SX=AMAX1(-50.,SX)
      GO TO 275
  290 IF (HCS.GT.TOL*HCT(3)) HCS=TOL*HCT(3)
  295 IF (NCR.EQ.1) HCS=HC/3.
      IF(HCS.GE.HCT(3).OR.HCS.LE.HCT(1)) HCS=(HCT(1)+HCT(3))/2.
      CALL SIM (HCS,XN,OS(1),INX)
  300 OT(2)=OS(1)
      HCT(2)=HCS
      NT=NN
      IF (KSS1.GT.2) GO TO 340
      SX=-SIG*20./FLOAT(NN)
      XNN=HC/RTO(NR)
      IF (NCR.EQ.1) GO TO 335
      IF (OZN(MR,NR).LT.1.1*OZP(LS)) XNS=XNN*0.5
      IF (OC(4).GT.OZP(LS)) XNS=XNN*0.5
      IF (XNS.EQ.XNN*0.5) GO TO 335
      DO 305 I=1,NCR
      J=NR+1-I
      OE(I+1)=OZN(MR,J)
  305 XNE(I+1)=RHO(MR,J)/F(J)
      OE(1)=OC(4)
      XNE(1)=0.
      NN=NCR+1
  310 IF (OE(NN).LT.OE(NN-1)) NN=NN-1
      IF (NN.EQ.1) XNS=XNN*0.5
      IF (NN.EQ.1) GO TO 335
      IF (OE(NN).LT.OE(NN-1)) GO TO 310
      IF (XNG.GE.XNE(2)) GO TO 320
      IF (ABS(XNE(2)-XNG).LT..0001) GO TO 325
      NN=NN+1
      NNR=NN-2
      DO 315 I=1,NNR
      II=NN-I+1
      XNE(II)=XNE(II-1)
  315 OE(II)=OE(II-1)
      XNE(2)=XNG
      OE(2)=OXN
      SX=-SIG*20./FLOAT(NN)
  320 IT=1
  325 CALL CURV1 (NN,OE,XNE,SP1,SP2,YP,TMP,SX)
      XNS=CURV2(OZP(LS),NN,OE,XNE,YP,SX,IT)
      IF (IT.GT.0) GO TO 330
      SX=SX*10.
      SX=AMAX1(-50.,SX)
      GO TO 325
  330 IF (XNS.GT.TOL*XNE(2)) XNS=TOL*XNE(2)
      IF(XNS.GE.XNE(3).OR.XNS.LE.XNE(1)) XNS=(XNE(1)+XNE(3))/2.
  335 IF (NCR.EQ.1) XNS=XN/3.
      CALL SIM (HC,XNS,OS(2),INX)
  340 RETURN
  345 WRITE (IOUT,350)
      STOP
C
C
C
  350 FORMAT (1H1,40HTHE LOWEST OZONE LINE CANNOT BE PLOTTED./1H0,39HINC
     1REASE THE MAXIMUM HC AND NOX VALUES.)
  355 FORMAT (1H1,24HNO LINES CAN BE PLOTTED./1H0,40HBACKGROUND ONLY PRO
     1DUCES TOO MUCH OZONE,,F3.2,5H PPM.)
  360 FORMAT (1H0,67HDUE TO HIGH BACKGROUND CONDITIONS THE LOWEST OZONE
     1PLOTTED WILL BE ,F3.2,5H PPM.)
  365 FORMAT (1H1,//,14X,36HTHE FOLLOWING SIMULATIONS WERE DONE./1H0/1H
     1,16X,2HHC,18X,3HNOX,15X,5HRATIO,16X,5HOZONE)
  370 FORMAT (1H1,//,14X,36HTHE FOLLOWING SIMULATIONS WERE DONE./1H0/1H
     1,16X,2HHC,18X,3HNOX,15X,5HRATIO,16X,5HOZONE,16X,4HTIME)
      END
```

# Subroutine SIM

```
      SUBROUTINE SIM (HC,XN,ZN,INX)
      COMMON /CALC/ NR,KR(77,5),A(77),S(77),R(77),ITYPE(77),IA(34),JA(21
     18),DILUT,TEMP,ERR,START,STOPP,SPECIS(34),TPRNT,TSTEP
      COMMON /TITL/ ITTL(18)
      COMMON /HOUR/ OZM,NGO,TM
      COMMON /CNTRL/ SIG,SIGMA,INFO,NPTO,XNF,RCTY,ALDX,OZIN,OZAL,HCIN,HC
     1AL,XNIN,XNAL,TSRT,DTIM,Z1,Z2,DCON,EHC,EXN,FLST,TLST
      COMMON /INOUT/ IN,IOUT,ITAPE
      COMMON /PHOTON/ CF(45,8),P(15,9),IPH(9)
      DIMENSION C(34), RT(77), XR(8)
      DATA IN1/1/
      START=0.
      T=START
      FLST=1.0
      TLST=START
      TCI=800.
      EHC=HC
      EXN=XN
      IF (IN1.EQ.1) SAV=STOPP
      STOPP=SAV
      IF (NPTO.EQ.0) TPRNT=STOPP
      IN1=0
      H=1.E-10
      NS=33
      N=33
      M=32
      DO 5 I=1,N
    5 C(I)=0.
      C(1)=XN*XNF+XNIN
      C(2)=XN*(1.-XNF)
      C(4)=OZIN
      C(12)=(HC*RCTY+HCIN*0.1)/3.
      C(21)=HC*.4*ALDX
      C(22)=HC*.3*ALDX
      C(24)=(HC*(1.-RCTY)+HCIN*0.9)*0.25
      IN=1
      CALL DIFSET (N,START,C,RT)
      IF (NPTO.EQ.0) GO TO 10
      CALL ISOPLT (HC,XN)
      WRITE (IOUT,125)
      WRITE (IOUT,135) (ITTL(I),I=1,18)
      IF (INFO.LT.1) WRITE (IOUT,170)
      IF (INFO.LT.1) GO TO 10
      WRITE (IOUT,150) ERR
      WRITE (IOUT,155) (R(IR),IR=1,NR)
      WRITE (IOUT,160) (IPH(IR),IR=1,8)
      DO 8 I=1,8
      J=IPH(I)
    8 XR(I)=R(J)
      WRITE (IOUT,165) (XR(IR),IR=1,8)
   10 DILUT=DCON
      IF (TSRT.LE.START.AND.DTIM.NE.0.) DILUT=ALOG(Z2/Z1)/DTIM
      TNEXT=1.
      IF (NPTO.EQ.0) GO TO 50
      IF (T-START) 75,75,50
   15 IF (DTIM.EQ.0.) GO TO 45
      IF (T.GE.TSRT) GO TO 30
      DILUT=DCON
      IF (TSRT-TPRNT) 20,20,25
   20 TNEXT=TSRT
      IN=2
      GO TO 50
   25 TNEXT=TPRNT
      IN=0
      GO TO 50
   30 IF (T.GE.TSRT+DTIM) GO TO 45
      DILUT=ALOG(Z2/Z1)/DTIM
      FLST=EXP(-DCON*TSRT)
      TLST=TSRT
      TNEXT=TSRT+DTIM
      IF (TNEXT-TPRNT) 35,35,40
   35 IN=2
      GO TO 50
   40 TNEXT=TPRNT
      IN=0
      GO TO 50
   45 TNEXT=AMIN1(TPRNT,STOPP)
      FLST=EXP(-DCON*TSRT-DILUT*DTIM)
      TLST=TSRT+DTIM
      DILUT=DCON
   50 CALL DRIVES (M,T,H,C,TNEXT,ERR,21,IN,IA,JA)
      T=TNEXT
      IF (NPTO.NE.0) GO TO 60
      IF (T.LT.STOPP) GO TO 15
      IF (INX.GT.-1) GO TO 60
      IF (INX.EQ.-1.AND.OZM.GT.0.75*ZN) GO TO 60
      IF (INX.NE.-2) GO TO 55
      IF (OZM.LT.1.25*ZN.AND.OZM.GT.0.75*ZN) GO TO 60
   55 ZN=OZM
      RETURN
   60 ZN=OZM
      IF (NPTO.NE.0) GO TO 70
      INX=1
      IF (T.LT.STOPP) GO TO 15
      IF (XN.EQ.0.) RR=0.
      IF (XN.NE.0.) RR=HC/XN
      IF (INFO.LT.0) GO TO 65
      IF (TM.GT.0.) WRITE (IOUT,100) HC,XN,RR,ZN
      IF (TM.LE.0.) WRITE (IOUT,120) HC,XN,RR,ZN
      RETURN
   65 IF (TM.GT.0.) WRITE (IOUT,140) HC,XN,RR,ZN,TM
      IF (TM.LT.0.) WRITE (IOUT,145) HC,XN,RR,ZN
      RETURN
   70 IF (IN.NE.0) RETURN
      IF (T.GE.STOPP) TPRNT=STOPP
      IF (T.LT.TPRNT) GO TO 15
   75 HCC=3.0*C(12)+4.0*C(24)
      IF (HCC.GT.0.0000001) GO TO 80
      FPROP=0.
      ALDC=0.
      GO TO 85
   80 FPROP=3.0*C(12)/HCC
      ALDC=(C(21)+2.0*C(22))/HCC
   85 CNOX=C(1)+C(2)
```

```
      IF (CNOX.LE.0.0000001) FNO2=0.
      IF (CNOX.GT.0.0000001) FNO2=C(1)/CNOX
      CO3=C(4)
      IF (INFO.GT.0) WRITE (IOUT,125)
      IF (INFO.GT.0) WRITE (IOUT,170)
      IF (T.EQ.START) TIMNW=START
      IF (T.NE.START) TIMNW=TPRNT
      CTIME=CLOCK(TCI,IFIX(TIMNW))
      WRITE (IOUT,175) CTIME,HCC,FPROP,ALDC,CNOX,FNO2,CO3
      IF (INFO.LE.0) GO TO 95
      WRITE (IOUT,115) (SPECIS(I),I=1,ND)
      WRITE (IOUT,130) CTIME,(C(I),I=1,10),H,(C(I),I=11,ND)
      CALL DIFFUN (N,TIMNW,C,RT)
      WRITE (IOUT,105) (RT(I),I=1,ND)
      DO 90 I=1,NR
      J=KR(I,1)
      K=KR(I,2)
      IF (J.EQ.0) RT(I)=0.
      IF (J.EQ.0) GO TO 90
      IF (J.EQ.99) J=0
      IF (J.EQ.0) TJ=1.
      IF (J.NE.0) TJ=C(J)
      IF (K.EQ.0) TK=1.
      IF (K.NE.0) TK=C(K)
      RT(I)=TJ*TK*R(I)
   90 CONTINUE
      WRITE (IOUT,110) (RT(I),I=1,NR)
      DO 91 IR=1,8
      J=IPH(IR)
   91 XR(IR)=R(J)
      WRITE (IOUT,165) (XR(IR),IR=1,8)
   95 IF (TIMNW.EQ.START) GO TO 50
      IF (NPTO.NE.0) IN1=1
      IF (T.GE.STOPP) RETURN
      TPRNT=TPRNT+TSTEP
      GO TO 15
C
C
  100 FORMAT (1H0,4F20.5)
  105 FORMAT (/,10H NET RATES,1X,1P10E12.3,/,(11X,1P10E12.3))
  110 FORMAT (//,1X,22HTHE REACTION RATES ARE,/,(1H ,1P10E13.2))
  115 FORMAT (//,3X,5HTIME ,4X,10(4X,A4,4X),/,1X,8HINTERVAL,3X,10(4X,A4,
     14X),/,(12X,10(4X,A4,4X)))
  120 FORMAT (1H0,4F20.5,8H NOT MAX)
  125 FORMAT (1H1//////////)
  130 FORMAT (1PE11.3,10E12.3/,E11.3,10E12.3/,(11X,10E12.3))
  135 FORMAT (46X,18A4)
  140 FORMAT (1H0,4F20.5,F21.0)
  145 FORMAT (1H0,4F20.5,14X,7HNOT MAX)
  150 FORMAT (24H0THE ERROR TOLERANCE IS ,1PE10.3)
  155 FORMAT (29H0THE RATE CONSTANTS USED WERE,//,(1H0,1P10E13.3))
  160 FORMAT (29H0THE PHOTOLYSIS REACTIONS ARE,/(1H0,9I13))
  165 FORMAT (34H0THE PHOTOLYTIC RATE CONSTANTS ARE,/,(1H0,4X,1P9E13.3))
  170 FORMAT (1H0,30X,4HTIME,6X,2HHC,7X,9HPROPYLENE,5X,8HALDEHYDE,6X,3HN
     10X,10X,3HNO2,8X,5HOZONE,/,30X,6H(LDT ),4X,5HTOTAL,5X,8HFRACTION,6X
     2,8HFRACTION,5X,5HTOTAL,7X,8HFRACTION,3X,9H(INSTANT))
  175 FORMAT (1H0,28X,F6.0.1X,F10.5,2X,F10.5,3X,F10.5,1X,F10.5,3X,F10.5,
     12X,F10.5)
      END
```

## Subroutine DRIVES

```
      SUBROUTINE DRIVES (N,T0,H0,Y0,TOUT,EPS,MF,INDEX,IA,JA)
      DIMENSION Y(032,06), IA(1), JA(1), Y0(N)
      COMMON /CNTRL/ SIG,SIGMA,INFO,NPTO,XNF,RCTY,ALDX,OZIN,OZAL,HCIN,HC
     1AL,XNIN,XNAL,TSRT,DTIM,Z1,Z2,DCON,EHC,EXN,FLST,TLST
      COMMON /GEAR1/ T,H,HMIN,HMAX,EPSC,UROUND,NC,MFC,KFLAG,JSTART
      COMMON /GEAR2/ YMAX(032)/GEAR3/ERROR(32)/GEAR4/W1(32,3)
      COMMON /GEAR5/ IW1(33,9)/GEAR6/W2(1500)/GEAR7/IW2(660)
      COMMON /GEAR8/ EPSJ,IPTI2,IPTI3,IPTI4,IPTR2,IPTR3,NGRP
      COMMON /GEAR9/ HUSED,NQUSED,NSTEP,NFE,NJE,NZA,NPL,NPU,NZL,NZU,NZRO
      COMMON /INOUT/ INP,LOUT,ITAPE
      DATA NMX/032/,LENW2/1500/,LENIW2/660/
      DATA UROUND/7.5E-9/
      KOZ=4
      NGP=0
      IF (INDEX.EQ.4) GO TO 5
      IF (INDEX.EQ.0) GO TO 20
      IF (INDEX.EQ.2) GO TO 25
      IF (INDEX.EQ.-1) GO TO 30
      IF (INDEX.EQ.3) GO TO 35
      IF (EPS.LE.0.) GO TO 105
      MITER=MF-10*(MF/10)
      IF ((MITER.NE.1).AND.(MITER.NE.2)) GO TO 5
      NP1=N+1
      NZA=IA(NP1)-1
      IPTI2=NZA+1
      MAXPL=(LENIW2-NZA)/2
      IPTI3=IPTI2+MAXPL
      NPL=IW1(N,4)
      NPU=IW1(N,6)
      NZL=IW1(N+1,3)
      NZU=IW1(N+1,5)
      IPTR2=NZA+1
      IPTR3=IPTR2+MAX0(NZA,NZL)
    5 DO 10 I=1,N
      YMAX(I)=ABS(Y0(I))
      IF (YMAX(I).EQ.0.) YMAX(I)=1.E-10
   10 Y(I,1)=Y0(I)
      NC=N
      T=T0
      H=H0
      NZRO=0
      TST=EPS*1.E-10
      DO 15 I=1,N
   15 IF (Y(I,1).GT.TST) NZRO=NZRO+1
      NZRO=MAX0(NZRO,1)
      NOLD=NZRO
      HMIN=ABS(H0)
      HMAX=ABS(T0-TOUT)*10.
      HMAX=AMIN1(HMAX,20.)
      EPSC=EPS
      MFC=MF
      JSTART=0
      N0=N
      CALL OZMX (Y,TL,TOUT,N0)
      NMX1=NMX+1
      EPSJ=SQRT(UROUND)
      NHCUT=0
      GO TO 40
   20 HMAX=ABS(TOUT-TOUTP)*10.
      HMAX=AMIN1(HMAX,20.)
      GO TO 65
   25 HMAX=ABS(TOUT-TOUTP)*10.
      HMAX=AMIN1(HMAX,20.)
      IF ((T-TOUT)*H.GE.0.) GO TO 110
      GO TO 70
   30 JSTART=-1
      NC=N
      EPSC=EPS
      MFC=MF
   35 CONTINUE
   40 CALL STIFFS (Y,N0,IA,JA,W1,NMX,IW1,NMX1)
      IF (NPTO.NE.0) CALL SAVLIN (T,Y(KOZ,1))
      KGO=1-KFLAG
      GO TO (45,80,95,85),KGO
   45 CONTINUE
      IF (T.GE.TL) CALL OZMX (Y,TL,TOUT,N0)
      D=0.
      NZRO=0
      DO 60 I=1,N
      IF (Y(I,1).GE.0.) GO TO 55
      NGP=NGP+1
      DO 50 J=1,6
   50 Y(I,J)=0.
   55 CONTINUE
      IF (Y(I,1).GT.TST) NZRO=NZRO+1
      AYI=ABS(Y(I,1))
      YMAX(I)=AMAX1(1.E-10,AYI)
   60 D=D+(AYI/YMAX(I))**2
      NZRO=MAX0(NZRO,1)
      IF (NZRO.NE.NOLD) JSTART=-1
      D=D*(UROUND/EPS)**2
      IF (D.GT.FLOAT(N)) GO TO 100
      IF (INDEX.EQ.3) GO TO 110
      IF (INDEX.EQ.2) GO TO 70
   65 IF ((T-TOUT)*H.LT.0.) GO TO 35
      CALL INTERP (TOUT,Y,N0,Y0)
      GO TO 120
   70 IF (T.GE.TOUT) GO TO 75
      IF (((T+H)-TOUT).LE.0.) GO TO 35
      H=(TOUT-T)*(1.+4.*UROUND)
      JSTART=-1
      GO TO 35
   75 JSTART=-1
      H=AMIN1(H,1.)
      GO TO 110
   80 CONTINUE
   85 IF (NHCUT.EQ.10) GO TO 90
      NHCUT=NHCUT+1
      HMIN=.1*HMIN
      H=.1*H
      JSTART=-1
      GO TO 35
   90 WRITE (LOUT,125)
      IF (KGO.EQ.4) WRITE (LOUT,140) T
      STOP
   95 WRITE (LOUT,130) T,H
      STOP
  100 WRITE (LOUT,135) T
      KFLAG=-2
      STOP
  105 WRITE (LOUT,145)
      STOP
  110 TOUT=T
      DO 115 I=1,N
  115 Y0(I)=Y(I,1)
  120 INDEX=KFLAG
      TOUTP=TOUT
      H0=HUSED
      IF (KFLAG.NE.0) H0=H
      RETURN
C
C
  125 FORMAT (//44H PROBLEM APPEARS UNSOLVABLE WITH GIVEN INPUT//)
  130 FORMAT (//35H KFLAG = -2 FROM INTEGRATOR AT T = ,E16.8,5H  H =,E16
     1.8/52H THE REQUESTED ERROR IS SMALLER THAN CAN BE HANDLED//)
  135 FORMAT (//37H INTEGRATION HALTED BY DRIVER AT T = ,E16.8/56H  EPS
     1TOO SMALL TO BE ATTAINED FOR THE MACHINE PRECISION/)
  140 FORMAT (//35H KFLAG = -3 FROM INTEGRATOR AT T = ,E16.8/45H  CORREC
     1TOR CONVERGENCE COULD NOT BE ACHIEVED/)
  145 FORMAT (//28H ILLEGAL INPUT.. EPS .LE. 0.//)
      END
```

## Subroutine STIFFS

```
      SUBROUTINE STIFFS (Y,N0,IA,JA,W1,NMX,IW1,NMX1)
      COMMON /GEAR1/ T,H,HMIN,HMAX,EPS,UROUND,N,MF,KFLAG,JSTART
      COMMON /GEAR2/ YMAX(032)/GEAR3/ERROR(32)
      COMMON /GEAR6/ W2(1500) /GEAR7/ IW2(660)
      COMMON /GEAR8/ EPSJ,IPTI2,IPTI3,IPTI4,IPTR2,IPTR3,NGRP
      COMMON /GEAR9/ HUSED,NQUSED,NSTEP,NFE,NJE,IDUMMY(5),NZRO
      COMMON /CALC/ NR,KR(77,5),A(77),S(77),R(77),ITYPE(77),II(34),JJ(21
     18),DILUT,TEMP,ERR,START,STOPP,SPECIS(34),TPRNT,TSTEP
      DIMENSION Y(N0,1), IA(1), JA(1), W1(NMX,1), IW1(NMX1,1)
      DIMENSION EL(13), TQ(4), RT(3)
      DATA EL(2)/1./,OLDL0/1./
      KFLAG=0
      TOLD=T
      IF (JSTART.GT.0) GO TO 50
      IF (JSTART.NE.0) GO TO 10
      CALL DIFFUN (N,T,Y,W1)
      DO 5 I=1,N
    5 Y(I,2)=H*W1(I,1)
      METH=MF/10
      MITER=MF-10*METH
      NQ=1
      L=2
      IDOUB=3
      RMAX=1.E4
      RC=0.
      CRATE=1.
      HOLD=H
      MFOLD=MF
      NSTEP=0
      NSTEPJ=0
      NFE=1
      NJE=0
      IRET=3
      GO TO 15
   10 IF (MF.EQ.MFOLD) GO TO 25
      MEO=METH
      MIO=MITER
      METH=MF/10
      MITER=MF-10*METH
      MFOLD=MF
      IF (MITER.NE.MIO) IWEVAL=MITER
      IF (METH.EQ.MEO) GO TO 25
      IDOUB=L+1
      IRET=1
   15 CALL COSET (METH,NQ,EL,TQ,MAXDER)
      LMAX=MAXDER+1
      RC=RC*EL(1)/OLDL0
      OLDL0=EL(1)
   20 FN=FLOAT(NZRO)
      EDN=FN*(TQ(1)*EPS)**2
      E=FN*(TQ(2)*EPS)**2
      EUP=FN*(TQ(3)*EPS)**2
      BND=FN*(TQ(4)*EPS)**2
      EPSOLD=EPS
      NOLD=NZRO
      GO TO (30,35,50),IRET
   25 IF(EPS.EQ.EPSOLD.AND.NZRO.EQ.NOLD) GO TO 30
```

```
      IRET=1
      GO TO 20
   30 IF (H.EQ.HOLD) GO TO 50
      RH=H/HOLD
      H=HOLD
      IREDO=3
      GO TO 40
   35 RH=AMAX1(RH,HMIN/ABS(H))
   40 RH=AMIN1(RH,HMAX/ABS(H),RMAX)
      R1=1.
      DO 45 J=2,L
      R1=R1*RH
      DO 45 I=1,N
   45 Y(I,J)=Y(I,J)*R1
      H=H*RH
      RC=RC*RH
      IDOUB=L+1
      IF (IREDO.EQ.0) GO TO 290
   50 IF (ABS(RC-1.).GT.0.3) IWEVAL=MITER
      IF (NSTEP.GE.NSTEPJ+20) IWEVAL=MITER
      T=T+H
      DO 55 J1=1,NQ
      DO 55 J2=J1,NQ
      J=(NQ+J1)-J2
      DO 55 I=1,N
   55 Y(I,J)=Y(I,J)+Y(I,J+1)
   60 DO 65 I=1,N
   65 ERROR(I)=0.
      M=0
      CALL DIFFUN (N,T,Y,W1(1,2))
      NFE=NFE+1
      IF (IWEVAL.LE.0) GO TO 130
      IWEVAL=0
      RC=1.
      NJE=NJE+1
      NSTEPJ=NSTEP
      CON=-H*EL(1)
      ISV=M
      LSV=L
      NZ=IA(N+1)-1
      DO 75 I=1,NZ
   75 W2(I)=0.
      DO 115 IR=1,NR
      MT=ITYPE(IR)
      DO 80 I=1,MT
      JX=I+1-I/2*2
      J=KR(IR,JX)
      IF (J.EQ.0) XX=1.
      IF (J.GT.0) XX=Y(J,1)
   80 RT(I)=R(IR)*XX
      DO 110 K=1,MT
      I=KR(IR,K)
      DO 90 L=1,MT
      J=KR(IR,L)
      M=IA(J)-1
   85 M=M+1
      IF (I-JA(M)) 85,90,85
   90 W2(M)=W2(M)-RT(L)
      DO 105 L=3,5
      J=KR(IR,L)
      M=IA(I)-1
      IF (J) 105,110,95
   95 M=M+1
      IF (J-JA(M)) 95,100,95
  100 W2(M)=W2(M)+RT(K)
  105 CONTINUE
  110 CONTINUE
  115 CONTINUE
      DO 125 J=1,N
      KMIN=IA(J)
      KMAX=IA(J+1)-1
      DO 120 K=KMIN,KMAX
      W2(K)=W2(K)*CON
      IF (JA(K).EQ.J) W2(K)=W2(K)+1.-CON*DILUT
  120 CONTINUE
  125 CONTINUE
      CALL NSCORA (N,IA,JA,W2,IW1(1,2),W2(IPTR3),W2(IPTR2),IW1,IW1(1,7),
     1IW1(1,8))
      CALL NSNFAC (N,IW1(1,2),IW2,W2,IW1(1,3),IW2(IPTI2),IW1(1,4),W2(IPT
     1R2),W1(1,3),IW1(1,5),IW2(IPTI3),IW1(1,6),W2(IPTR3),W1,IW1(1,7),IW1
     2(1,8),IER)
      M=ISV
      L=LSV
      IF (IER.NE.0) GO TO 160
  130 DO 135 I=1,N
      IF (M.LE.0) GO TO 135
      IF (-H*W1(I,2)*10..GT.Y(I,1)) GO TO 155
  135 W1(I,1)=H*W1(I,2)-(Y(I,2)+ERROR(I))
      CALL NSBSLV (N,IW1,IW1,IW1(1,3),IW2(IPTI2),IW1(1,4),W2(IPTR2),W1(1
     1,3),IW1(1,5),IW2(IPTI3),IW1(1,6),W2(IPTR3),W1(1,2),W1,W2)
      D=0.
      DO 145 I=1,N
      ERROR(I)=ERROR(I)+W1(I,2)
      D=D+(W1(I,2)/YMAX(I))**2
  145 W1(I,1)=Y(I,1)+EL(1)*ERROR(I)
      IF (M.NE.0) CRATE=AMAX1(.9*CRATE,D/D1)
      IF ((D*AMIN1(1.,2.*CRATE)).LE.BND) GO TO 175
      D1=D
      M=M+1
      IF (M.EQ.3) GO TO 155
      CALL DIFFUN (N,T,W1,W1(1,2))
      GO TO 130
  155 NFE=NFE+2
      IF (IWEVAL.EQ.-1) GO TO 170
  160 T=TOLD
      RMAX=2.
      DO 165 J1=1,NQ
      DO 165 J2=J1,NQ
      J=(NQ+J1)-J2
      DO 165 I=1,N
  165 Y(I,J)=Y(I,J)-Y(I,J+1)
      IF (ABS(H).LE.HMIN*1.00001) GO TO 285
      RH=.25
      IREDO=1
      GO TO 35
  170 IWEVAL=MITER
      GO TO 60
  175 IF (MITER.NE.0) IWEVAL=-1
      NFE=NFE+M
      D=0.
      DO 180 I=1,N
  180 D=D+(ERROR(I)/YMAX(I))**2
      IF (D.GT.E) GO TO 195
      KFLAG=0
      IREDO=0
      NSTEP=NSTEP+1
      HUSED=H
      NQUSED=NQ
      DO 185 J=1,L
      DO 185 I=1,N
  185 Y(I,J)=Y(I,J)+EL(J)*ERROR(I)
      IF (IDOUB.EQ.1) GO TO 205
      IDOUB=IDOUB-1
      IF (IDOUB.GT.1) GO TO 295
      IF (L.EQ.LMAX) GO TO 295
      DO 190 I=1,N
  190 Y(I,LMAX)=ERROR(I)
      GO TO 295
  195 KFLAG=KFLAG-1
      T=TOLD
      DO 200 J1=1,NQ
      DO 200 J2=J1,NQ
      J=(NQ+J1)-J2
      DO 200 I=1,N
  200 Y(I,J)=Y(I,J)-Y(I,J+1)
      RMAX=2.
      IF (ABS(H).LE.HMIN*1.00001) GO TO 275
      IF (KFLAG.LE.-3) GO TO 265
      IREDO=2
      PR3=1.E+20
      GO TO 215
  205 PR3=1.E+20
      IF (L.EQ.LMAX) GO TO 215
      D1=0.
      DO 210 I=1,N
  210 D1=D1+((ERROR(I)-Y(I,LMAX))/YMAX(I))**2
      ENQ3=.5/FLOAT(L+1)
      PR3=((D1/EUP)**ENQ3)*1.4+1.4E-6
  215 ENQ2=.5/FLOAT(L)
      PR2=((D/E)**ENQ2)*1.2+1.2E-6
      PR1=1.E+20
      IF (NQ.EQ.1) GO TO 225
      D=0.
      DO 220 I=1,N
  220 D=D+(Y(I,L)/YMAX(I))**2
      ENQ1=.5/FLOAT(NQ)
      PR1=((D/EDN)**ENQ1)*1.3+1.3E-6
  225 IF (PR2.LE.PR3) GO TO 230
      IF (PR3.LT.PR1) GO TO 240
      GO TO 235
  230 IF (PR2.GT.PR1) GO TO 235
```

```
      NEWQ=NQ
      RH=1./PR2
      GO TO 255
  235 NEWQ=NQ-1
      RH=1./PR1
      GO TO 255
  240 NEWQ=L
      RH=1./PR3
      IF (RH.LT.1.1) GO TO 250
      DO 245 I=1,N
  245 Y(I,NEWQ+1)=ERROR(I)*EL(L)/FLOAT(L)
      GO TO 260
  250 IDOUB=10
      GO TO 295
  255 IF ((KFLAG.EQ.0).AND.(RH.LT.1.1)) GO TO 250
      IF (NEWQ.EQ.NQ) GO TO 35
  260 NQ=NEWQ
      L=NQ+1
      IRET=2
      GO TO 15
  265 IF (KFLAG.EQ.-9) GO TO 280
      RH=10.**KFLAG
      RH=AMAX1(HMIN/ABS(H),RH)
      H=H*RH
      CALL DIFFUN (N,T,Y,W1)
      NFE=NFE+1
      DO 270 I=1,N
  270 Y(I,2)=H*W1(I,1)
      IWEVAL=MITER
      IDOUB=10
      IF (NQ.EQ.1) GO TO 50
      NQ=1
      L=2
      IRET=3
      GO TO 15
  275 KFLAG=-1
      GO TO 295
  280 KFLAG=-2
      GO TO 295
  285 KFLAG=-3
      GO TO 295
  290 RMAX=100.
  295 HOLD=H
      JSTART=NQ
      RETURN
      END
```

## Subroutine DIFFUN

```
      SUBROUTINE DIFFUN (L,T,X,XT)
      COMMON /CALC/ NR,KR(77,5),A(77),S(77),R(77),ITYPE(77),IA(34),JA(21
     18),DILUT,TEMP,ERR,START,STOPP,SPECIS(34),TPRNT,TSTEP
      COMMON /CNTRL/ SIG,SIGMA,INFO,NPTO,XNF,RCTY,ALDX,OZIN,OZAL,HCIN,HC
     1AL,XNIN,XNAL,TSRT,DTIM,Z1,Z2,DCON,EHC,EXN,FLST,TLST
      COMMON /EMIS/ NEM,EM(11),EMHC(11),EMNOX(11),ESTRT(2),ESTOP,ESLP,EH
     1SLP,ENSLP,B(2),EC(36),BB(2),EH(36),CC(2),EX(36)
      COMMON /PHOTON/ CF(45,8),P(15,9),IPH(9)
      DIMENSION XT(L), X(L)
      N=L
      DILU=AMAX1(DILUT,0.)
      DO 5 I=1,N
    5 XT(I)=-DILU*X(I)
      IF (T.LT.TSRT.OR.T.GT.TSRT+DTIM) GO TO 10
      XT(1)=DILU*(XNAL-X(1))
      XT(4)=DILU*(OZAL-X(4))
      XT(12)=DILU*(0.03333333*HCAL-X(12))
      XT(24)=DILU *(0.225*HCAL-X(24))
   10 IF (T.GE.ESTOP) GO TO 25
      FNOW=FLST*EXP(-DILUT*(T-TLST))
      IF (T.GT.60.) GO TO 15
      ENOW=0.
      IF (NEM.GT.0) ENOW=(ESTRT(1)+T*ESLP)*FNOW
      ENOW1=ENOW
      ENOW2=ENOW
      IF (NEM.LE.-1.AND.EMHC(1).GE.-0.) ENOW1=(ESTRT(1)+T*EHSLP)*FNOW
      IF (NEM.LE.-1.AND.EMNOX(1).GE.-0.) ENOW2=(ESTRT(2)+T*ENSLP)*FNOW
      GO TO 20
   15 I=IFIX(T/60.)
      ENOW=0.
      IF (NEM.GT.0) ENOW=(((T*EC(4*I)+EC(4*I-1))*T+EC(4*I-2))*T+EC(4*I-3
     1))*FNOW
      ENOW1=ENOW
      ENOW2=ENOW
      IF (NEM.LE.-1.AND.EMHC(1).GE.-0.) ENOW1=(((T*EH(4*I)+EH(4*I-1))*T+
     1EH(4*I-2))*T+EH(4*I-3))*FNOW
      IF (NEM.LE.-1.AND.EMNOX(1).GE.-0.) ENOW2=(((T*EX(4*I)+EX(4*I-1))*T
     1+EX(4*I-2))*T+EX(4*I-3))*FNOW
   20 XT(1)=XT(1)+ENOW2*EXN*0.1
      XT(2)=XT(2)+ENOW2*EXN*0.9
      XT(12)=XT(12)+ENOW1*EHC*RCTY/3.
      XT(21)=XT(21)+ENOW1*EHC*ALDX*.4
      XT(22)=XT(22)+ENOW1*EHC*ALDX*.3
      XT(24)=XT(24)+ENOW1*EHC*(1.-RCTY)*0.25
   25 IF (T.EQ.TOLD) GO TO 35
      I=IFIX(T/60.+2.001)
      IF (I.GT.16) I=16
      Z=T/60.-FLOAT(I-2)
      DO 30 J=1,8
      IR=IPH(J)
      IF (P(I-1,J).EQ.0.) R(IR)=0.
      IF (P(I-1,J).EQ.0.) GO TO 30
      R(IR)=((Z*CF(3*I-3,J)+CF(3*I-4,J))*Z+CF(3*I-5,J))*Z+P(I-1,J)
   30 IF (R(IR).LT.0.) R(IR)=0.
   35 DO 55 IR=1,NR
      I=KR(IR,1)
      IF (ITYPE(IR).EQ.2) GO TO 40
      RT=R(IR)*X(I)
      GO TO 45
   40 J=KR(IR,2)
      RT=R(IR)*X(I)*X(J)
      XT(J)=XT(J)-RT
   45 XT(I)=XT(I)-RT
      DO 50 K=3,5
      I=KR(IR,K)
      IF (I.EQ.0) GO TO 55
   50 XT(I)=XT(I)+RT
   55 CONTINUE
      TOLD=T
      RETURN
C     ENTRY DIFSET
      ENTRY DIFSET (L,T,X,XT)
      TOLD=T
      I=2
      Z=1./60.
      DO 60 J=1,8
      IR=IPH(J)
   60 R(IR)=P(I,J)
      RETURN
      END
```

## Subroutine OZMX

```
      SUBROUTINE OZMX (C,TL,TOUT,N0)
C
      DIMENSION C(N0,6), RUN(61), OZ(61)
      COMMON /GEAR1/ T,H,HMIN,HMAX,EPSC,UROUND,NC,MFC,KFLAG,JSTART
      COMMON /HOUR/ OZM,NCO,TM
      COMMON /CALC/ NR,KR(77,5),A(77),S(77),R(77),ITYPE(77),IA(34),JA(21
     18),DILUT,TEMP,ERR,START,STOPP,SPECIS(34),TPRNT,TSTEP
      NQ=JSTART
      IF (T.NE.START) GO TO 5
      KOZ=4
      RUN(1)=C(KOZ,1)
      NT=1
      TL=START+1.
      OZM=0.
      OZA=0.
      RETURN
    5 DO 10 I=1,61
      RR=(TL+FLOAT(I-1)-T)/H
      IF (RR.GT.0.) GO TO 15
      IF (TL+FLOAT(I-1).GT.STOPP) GO TO 15
      OZ(I)=C(KOZ,1)
      RH=1.
      DO 10 J=1,NQ
      RH=RH*RR
   10 OZ(I)=OZ(I)+RH*C(KOZ,J+1)
      I=61
   15 I=I-1
      TL=TL+FLOAT(I)
      DO 35 J=1,I
      IF (NT.GT.60) GO TO 25
      RUN(NT+1)=OZ(J)
      NT=NT+1
      IF (NT.LT.61) GO TO 35
      SIX=0.
      S2=RUN(60)
      DO 20 K=1,29
      SIX=SIX+RUN(2*K+1)
   20 S2=S2+RUN(2*K)
   25 OZA=2.*SIX+4.*S2+RUN(1)+OZ(J)
      SV=SIX
      SIX=S2-RUN(2)
      S2=SV+OZ(J)
      RUN(61)=OZ(J)
      DO 30 K=1,60
   30 RUN(K)=RUN(K+1)
      IF (OZA.GT.OZM) OZM=OZA
      IF (OZA.EQ.OZM) TM=TL+FLOAT(J-I-31)
   35 CONTINUE
      IF (TL-T.LT.0..AND.T.LT.STOPP) GO TO 5
      IF (NCO.NE.0) GO TO 40
      IF (T.GT.360..AND.OZA.LT.OZM) GO TO 45
   40 IF (T.LT.STOPP) RETURN
      GO TO 50
   45 TOUT=T
      STOPP=T
   50 OZM=OZM/180.
      OZA=OZA/180.
      IF (OZA.LT.OZM) RETURN
      IF(T.GT.STOPP.AND.OZM.GT.0.00001) TM=-TM
      RETURN
      END
```

## Subroutine COSET

```
      SUBROUTINE COSET (METH,NQ,EL,TQ,MAXDER)
      DIMENSION PERTST(12,2,3), EL(13), TQ(4)
      DATA PERTST/1.,1.,2.,1.,.3158,.07407,.01391,.002182,.0002945,.0000
     13492,.000003692,.0000003524,1.,1.,.5,.1667,.04167,1.,1.,1.,1.,1.,1
     2.,1.,2.,12.,24.,37.89,53.33,70.08,87.97,106.9,126.7,147.4,168.8,19
     31.0,2.0,4.5,7.333,10.42,13.7,1.,1.,1.,1.,1.,1.,1.,12.0,24.0,37.89,
     453.33,70.08,87.97,106.9,126.7,147.4,168.8,191.0,1.,3.0,6.0,9.167,1
     52.5,1.,1.,1.,1.,1.,1.,1.,1./
    5 MAXDER=5
      GO TO (10,15,20,25,30),NQ
   10 EL(1)=1.0
      GO TO 35
   15 EL(1)=6.6666666666667E-01
      EL(3)=3.3333333333333E-01
      GO TO 35
   20 EL(1)=5.4545454545455E-01
      EL(3)=EL(1)
      EL(4)=9.0909090909091E-02
      GO TO 35
   25 EL(1)=0.48
      EL(3)=0.7
      EL(4)=0.2
      EL(5)=0.02
      GO TO 35
   30 EL(1)=4.3795620437956E-01
      EL(3)=8.2116788321168E-01
      EL(4)=3.1021897810219E-01
      EL(5)=5.4744525547445E-02
      EL(6)=3.6496350364964E-03
   35 DO 40 K=1,3
   40 TQ(K)=PERTST(NQ,METH,K)
      TQ(4)=.5*TQ(2)/FLOAT(NQ+2)
      RETURN
      END
```

## Subroutine NSCORA

```
      SUBROUTINE NSCORA (N,IA,JA,A,IAP,JAWORK,AWORK,C,IR,ICT)
      INTEGER IA(1),JA(1),IAP(1),JAWORK(1),C(1),IR(1),ICT(1)
      REAL A(1),AWORK(1)
      DO 5 K=1,N
      ICK=C(K)
    5 IR(ICK)=K
      JMIN=1
      DO 15 K=1,N
      ICK=C(K)
      JMAX=JMIN+IA(ICK+1)-IA(ICK)-1
      IF (JMIN.GT.JMAX) GO TO 15
      IAINK=IA(ICK)-1
      DO 10 J=JMIN,JMAX
      IAINK=IAINK+1
      JAOUTJ=JA(IAINK)
      JAOUTJ=IR(JAOUTJ)
      JAWORK(J)=JAOUTJ
   10 AWORK(J)=A(IAINK)
   15 JMIN=JMAX+1
      DO 20 I=1,N
   20 ICT(I)=IAP(I)
      JMIN=1
      DO 30 I=1,N
      ICK=C(I)
      JMAX=JMIN+IA(ICK+1)-IA(ICK)-1
      IF (JMIN.GT.JMAX) GO TO 30
      DO 25 J=JMIN,JMAX
      JAOUTJ=JAWORK(J)
      ICTJ=ICT(JAOUTJ)
      A(ICTJ)=AWORK(J)
      ICT(JAOUTJ)=ICTJ+1
   25 CONTINUE
   30 JMIN=JMAX+1
      RETURN
      END
```

## Subroutine NSNFAC

```
      SUBROUTINE NSNFAC (N,IA,JA,A,IL,JL,ISL,L,D,IU,JU,ISU,U,X,IRL,JRL,I
     1ER)
      INTEGER IA(1),JA(1),IL(1),JL(1),ISL(1)
      INTEGER IU(1),JU(1),ISU(1),IRL(1),JRL(1)
      REAL A(1),L(1),D(1),U(1),X(1)
      REAL LKI
      IER=0
      DO 5 K=1,N
      IRL(K)=IL(K)
    5 JRL(K)=0
      DO 95 K=1,N
      X(K)=0.
      I1=0
      IF (JRL(K).EQ.0) GO TO 15
      I=JRL(K)
   10 I2=JRL(I)
      JRL(I)=I1
      I1=I
      X(I)=0.
      I=I2
      IF (I.NE.0) GO TO 10
   15 JMIN=ISU(K)
      JMAX=JMIN+IU(K+1)-IU(K)-1
      IF (JMIN.GT.JMAX) GO TO 25
      DO 20 J=JMIN,JMAX
      JUJ=JU(J)
   20 X(JUJ)=0.
   25 JMIN=IA(K)
      JMAX=IA(K+1)-1
      DO 30 J=JMIN,JMAX
      JAJ=JA(J)
   30 X(JAJ)=A(J)
      I=I1
      IF (I.EQ.0) GO TO 50
   35 IRLI=IRL(I)
      LKI=-X(I)
      L(IRLI)=-LKI
      JMIN=IU(I)
      JMAX=IU(I+1)-1
      IF (JMIN.GT.JMAX) GO TO 45
      ISUB=ISU(I)-1
      DO 40 J=JMIN,JMAX
      ISUB=ISUB+1
      JUJ=JU(ISUB)
   40 X(JUJ)=X(JUJ)+LKI*U(J)
   45 I=JRL(I)
      IF (I.NE.0) GO TO 35
   50 IF (X(K).EQ.0.) GO TO 100
      DK=1./X(K)
      D(K)=DK
      IF (K.EQ.N) GO TO 95
      JMIN=IU(K)
      JMAX=IU(K+1)-1
      IF (JMIN.GT.JMAX) GO TO 60
      ISUB=ISU(K)-1
      DO 55 J=JMIN,JMAX
      ISUB=ISUB+1
      JUJ=JU(ISUB)
   55 U(J)=X(JUJ)*DK
   60 CONTINUE
      I=I1
      IF (I.EQ.0) GO TO 90
   70 IRL(I)=IRL(I)+1
      I1=JRL(I)
      IF (IRL(I).GE.IL(I+1)) GO TO 85
      ISLB=IRL(I)-IL(I)+ISL(I)
      J=JL(ISLB)
   75 IF (I.GT.JRL(J)) GO TO 80
      J=JRL(J)
      GO TO 75
   80 JRL(I)=JRL(J)
      JRL(J)=I
   85 I=I1
      IF (I.NE.0) GO TO 70
   90 ISLK=ISL(K)
      IF (IRL(K).GE.IL(K+1)) GO TO 95
      J=JL(ISLK)
      JRL(K)=JRL(J)
      JRL(J)=K
   95 CONTINUE
      RETURN
  100 IER=K
      RETURN
      END
```

# Subroutine NSBSLV

```
      SUBROUTINE NSBSLV (N,R,C,IL,JL,ISL,L,D,IU,JU,ISU,U,X,B,Y)
      DIMENSION R(1), IL(1), JL(1), IU(1), JU(1), C(1), ISL(1), ISU(1)
      DIMENSION L(1), X(1), B(1), U(1), Y(1), D(1)
      INTEGER R,RK,C,CK
      REAL L
      DO 5 K=1,N
      RK=R(K)
    5 Y(K)=B(RK)
      DO 15 K=1,N
      JMIN=IL(K)
      JMAX=IL(K+1)-1
      YK=-D(K)*Y(K)
      Y(K)=-YK
      IF (JMIN.GT.JMAX) GO TO 15
      ISLB=ISL(K)-1
      DO 10 J=JMIN,JMAX
      ISLB=ISLB+1
      JLJ=JL(ISLB)
   10 Y(JLJ)=Y(JLJ)+YK*L(J)
   15 CONTINUE
      K=N
      DO 30 I=1,N
      SUM=-Y(K)
      JMIN=IU(K)
      JMAX=IU(K+1)-1
      IF (JMIN.GT.JMAX) GO TO 25
      ISUB=ISU(K)-1
      DO 20 J=JMIN,JMAX
      ISUB=ISUB+1
      JUJ=JU(ISUB)
   20 SUM=SUM+U(J)*Y(JUJ)
   25 Y(K)=-SUM
      CK=C(K)
      X(CK)=-SUM
   30 K=K-1
      RETURN
      END
```

## Subroutine YSMER

```
      SUBROUTINE YSMER (A,K,A1)
      INTEGER A,A1(2)
      COMMON /INOUT/ INP,LOUT,ITAPE
      WRITE (LOUT,5) A,K,A1(1),A1(2)
      RETURN
C
    5 FORMAT (1X,A10,I6,2A10)
      END
```

## Subroutine INTERP

```
      SUBROUTINE INTERP (TOUT,Y,N0,Y0)
      COMMON /GEAR1/ T,H,DUMMY(4),N,IDUMMY(2),JSTART
      DIMENSION Y0(N0), Y(N0,1)
      DO 5 I=1,N
    5 Y0(I)=Y(I,1)
      L=JSTART+1
      S=(TOUT-T)/H
      S1=1.
      DO 15 J=2,L
      S1=S1*S
      DO 10 I=1,N
   10 Y0(I)=Y0(I)+S1*Y(I,J)
   15 CONTINUE
      RETURN
      END
```

## Subroutine LINER

```
      SUBROUTINE LINER (SIG,KALCMP,F)
      COMMON /NEED/ HC,XN,NL,NR,R(20),OZP(20),OZN(8,20),RHO(8,20),MR,OC(
     14),OS(2),HCS,XNS,LS,HCLL(8)
      COMMON /VVLBL/ FACTOR,DISTNC,CHRSZ,NCHR,OZLBL
      COMMON /PLTVEC/ HCT(20),OT(20),NT,OHC,HCG,PLTGRD,OXN,XNG,HCC,XNC,T
     1ICZ,DIGZ,CHRZ
      COMMON /CNTRL/ SGG,SIGMA,INFO,NPTO,XNF,RCTY,ALDX,OZIN,OZAL,HCIN,HC
     1AL,XNIN,XNAL,TSRT,DTIM,Z1,Z2,DCON,EHC,EXN,FLST,TLST
      COMMON /INOUT/ IN,IOUT,ITAPE
      COMMON /TITL/ ITTL(18)
      COMMON /GEAR6/ RPL(20,20),RTL(20,20),NRL(20),NSL(20),NTL(20),NUL(2
     10),W(20),WW(20),OE(20),HCTP(20),XNE(20),XNEP(20),YP(20),TM(20),XNA
     2P(20),HCAP(20),HCLP(20),ITTL1(18),U(44),V(44),DUM1(294)
      DIMENSION F(20), RBL(20,20), NBL(20), NTOL(20)
C
C  FIRST SET CALCOMP OPTION
C
      IF (KALCMP.LE.0) GO TO 5
      CHRSZ=TICZ
      IDIG1=1
      IDIG2=2
      IHY=IFIX(HC*10.+0.5)
      IHZ=IFIX(XN*1000.+0.5)
      IF (MOD(IHY,10).NE.0) IDIG1=2
      IF (MOD(IHZ,7).NE.0.OR.IHZ.LT.10) IDIG2=3
      HCC=HCC/HC
      HCX=0.
      HCM=HC/10.
      XNC=XNC/XN
      XNX=0.
      XNM=XN/7.
      XX=((10.0-(HCC*HC))/2.0)+0.3
      YY=((8.0-(XNC*XN))/2.0)+0.3
      ORGY=-.75
      CALL PLOTS (I1,I2,14)
      CALL PLOT (XX,YY,-3)
    5 M=MR+1
      NLL=0
      DO 10 I=1,NL
      NUL(I)=0
      NTL(I)=0
      NTOL(I)=0
      NBL(I)=0
      NSL(I)=0
   10 NRL(I)=0
      OE(1)=OC(4)
      OE(2)=OS(2)
      XNE(1)=0.
      XNE(2)=XNS
      DO 15 I=1,NR
      K=NR+1-I
      OE(I+2)=OZN(MR,K)
      XNE(I+2)=HC/R(K)
      IF (XNE(I+2).GT.XN) GO TO 20
   15 CONTINUE
      I=NR+1
```

```
20 I=I-1
   NE=I+2
   TOL=1.0-(0.17/(SQRT(FLOAT(NR))))
   NCR=(NR+1)/2
   CALL EDGMX (XNE,OE,NE,XMX,OZX,LX)
   NDIF=NE-LX+1
   NEW=NE
   NE=LX+1
   OE(NE)=OZX
   XNE(NE)=XMX
   CALL EDGMX (HCT,OT,NT,HMX,OZHX,LHX)
   NDIF1=NT-LHX+1
   NDIF2=NT-LHX-1
   NEW1=NT
   NT=LHX+1
   OT(NT)=OZHX
   HCT(NT)=HMX
   SX=-SIG*0.25
   IF (OZP(NL).LT.OC(2)) GO TO 30
   CALL NEWLIN (NT,OT,HCT,SX,LS,NL,1,0,HCTP,NPL,TOL,0,0,0)
   NTT=NPL
   IF (OZP(LS).GE.OC(2)) NLL=0
   IF (OZP(LS).GE.OC(2)) GO TO 50
30 SX=-SIG*10.
   IF (NR.GT.1) GO TO 35
   OT(1)=OC(1)
   HCT(1)=0.
   OT(2)=OC(2)
   HCT(2)=XN
   MR2=2
   GO TO 45
35 DO 40 II=1,MR
   OT(II+1)=OZN(II,1)
40 HCT(II+1)=HCLL(II)
   OT(1)=OC(1)
   HCT(1)=0.
   MR2=MR+1
45 CALL NEWLIN (MR2,OT,HCT,SX,LS,NL,2,0,HCLP,NLL,TOL,0,0,0)
   IF (OZP(NL).LT.OC(2)) NPL=NLL
50 NPLI=NPL+1
   IF (NPLI.GE.NL) GO TO 60
   DO 55 J=NPLI,NL
55 IF (OZP(J).LT.OE(NE)) NPL=NPL+1
60 SX=-SIG*10.
   CALL NEWLIN (NE,OE,XNE,SX,LS,NL,3,0,XNEP,NEL,TOL,0,0,0)
   IF (NDIF2.EQ.0) GO TO 75
   DO 65 II=LHX,NEW1
   JJ=LHX-II+1
   IF (IABS(JJ).GT.NCR) GO TO 70
   JO=II-LHX+1
   OT(JO)=OZN(MR,NCR+JJ-1)
65 HCT(JO)=R(NCR+JJ-1)*XN
70 OT(NDIF1)=OZHX
   HCT(NDIF1)=HMX
   SX=-SIG*10.
   CALL NEWLIN (NDIF1,OT,HCT,SX,NEL+1,NPL,4,NEL,HCAP,II,TOL,0,0,0)
75 IF ((NTT+NLL).GE.NPL) GO TO 90
```

```
      DO 80 II=LX,NEW
      JJ=II-LX+1
      IF (JJ.GT.NCR) GO TO 85
      OE(JJ)=OZN(MR,NCR+JJ-1)
   80 XNE(JJ)=HC/R(NCR+JJ-1)
   85 OE(NDIF)=OZX
      XNE(NDIF)=XMX
      SX=-SIG*10.
      CALL NEWLIN (NDIF,OE,XNE,SX,NTT+1,NPL,5,NTT,XNAP,II,TOL,0,0,0)
   90 IF (OZP(LS).LT.OC(2)) NR1=NR-1
      IF (OZP(LS).GE.OC(2)) NR1=NR
      NOZLST=0
      IF (OZP(LS).LT.OC(2)) IK=1
      IF (OZP(LS).GE.OC(2)) IK=0
      XOZ=AMAX1(OZHX,OZX,OC(3))
      IF (XOZ.EQ.OZHX) NOZLST=NT-2
      IF (XOZ.EQ.OC(3)) NOZLST=NCR
      IF (XOZ.EQ.OZX) NOZLST=NCR+NDIF-2
      DO 110 LL=1,NR1
      IF (OZP(LS).LT.OC(2)) I=LL+1
      IF (OZP(LS).GE.OC(2)) I=LL
      IF (NR.EQ.1) I=LL
      U(1)=OC(1)
      V(1)=0.
      DO 95 J=2,M
      U(J)=OZN(J-1,I)
   95 V(J)=RHO(J-1,I)
      SX=-SIG*3.0
      IF (M.GT.2) SX=-SIG*60./(FLOAT(M-2)**2)
      CALL EDGMX (V,U,M,HHMX,OZMMX,MM1)
      MM=MM1+1
      IF (MM.GE.M) GO TO 105
      U(MM)=OZMMX
      V(MM)=HHMX
      W(1)=OZN(MR,I)
      WW(1)=RHO(MR,I)
      MDIF=M-MM1+1
      DO 100 J=2,MDIF
      W(J)=OZN(M-J+1,I)
  100 WW(J)=RHO(M-J+1,I)
      W(MDIF)=OZMMX
      WW(MDIF)=HHMX
      IF ((LL-IK).LE.NOZLST) CALL NEWLIN (MDIF,W,WW,SX,LS,NL,6,0,RTL(1,I
     1),IJ,TOL,NUL,NTL,I)
      IF ((LL-IK).GT.NOZLST) CALL NEWLIN (MDIF,W,WW,SX,LS,NL,6,0,RBL(1,I
     1),IJ,TOL,NTOL,NBL,I)
      SX=-SIG*3.0
      IF (MM.GT.2) SX=-SIG*60./(FLOAT(MM-2)**2)
  105 CALL NEWLIN (MM,U,V,SX,LS,NL,7,0,RPL(1,I),II,TOL,NRL,NSL,I)
  110 CONTINUE
      CALL ISOPLT (HCTP,XN)
      SX=SIGMA*30./FLOAT(NR)
      NTT2=NTT+NLL
      IF (NTT.NE.0.AND.NLL.NE.0) NTT2=NTT
      NW=0
      DO 185 I=LS,NPL
      K=1
      IF (I.LE.NTT2) GO TO 115                                          T  168
      U(1)=HC                                                           T  169
      V(1)=XNAP(I-NTT)                                                  T  170
      GO TO 125                                                         T  171
  115 IF (OZP(LS).GT.OC(2)) GO TO 120                                   T  172
      IF (I.GT.NLL) GO TO 120                                           T  173
      U(1)=0.                                                           T  174
      V(1)=HCLP(I)                                                      T  175
      GO TO 125                                                         T  176
  120 U(1)=HCTP(I)                                                      T  177
      V(1)=XN                                                           T  178
  125 NT=NUL(I)                                                         T  179
      NE=NTL(I)                                                         T  180
      IF (NE.EQ.0) GO TO 135                                            T  181
      DO 130 JI=NE,NT                                                   T  182
      J=NT-JI+1                                                         T  183
      K=K+1                                                             T  184
      V(K)=RTL(I,J)/F(J)                                                T  185
  130 U(K)=V(K)*R(J)                                                    T  186
  135 NT=NRL(I)                                                         T  187
      NE=NSL(I)                                                         T  188
      IF (NE.EQ.0) GO TO 145                                            T  189
      DO 140 J=NE,NT                                                    T  190
      K=K+1                                                             T  191
      V(K)=RPL(I,J)/F(J)                                                T  192
  140 U(K)=V(K)*R(J)                                                    T  193
  145 NT=NTOL(I)                                                        T  194
      NE=NBL(I)                                                         T  195
      IF (NE.EQ.0) GO TO 155                                            T  196
      DO 150 JI=NE,NT                                                   T  197
      J=NT-JI+1                                                         T  198
      K=K+1                                                             T  199
      V(K)=RBL(I,J)/F(J)                                                T  200
  150 U(K)=V(K)*R(J)                                                    T  201
  155 IF (I.GT.NEL) GO TO 160                                           T  202
      K=K+1                                                             T  203
      U(K)=HC                                                           T  204
      V(K)=XNEP(I)                                                      T  205
      GO TO 165                                                         T  206
  160 IF (NDIF2.EQ.0) GO TO 165                                         T  207
      K=K+1                                                             T  208
      U(K)=HCAP(I-NEL)                                                  T  209
      V(K)=XN                                                           T  210
  165 U(K+1)=0.                                                         T  211
      U(K+2)=1./HCC                                                     T  212
      V(K+1)=0.                                                         T  213
      V(K+2)=1./XNC                                                     T  214
      IF (K.LE.2) GO TO 185                                             T  215
      OZLBL=OZP(I)                                                      T  216
      NW=NW+1                                                           T  216A
      W(NW)=OZP(I)                                                      T  216B
      NCHR=4                                                            T  217
      NCNT=0                                                            T  218
  170 VAL=OZLBL*(10.**NCNT)                                             T  219
      IF (VAL.GT.0.01) GO TO 175                                        T  220
      NCNT=NCNT+1                                                       T  221
      GO TO 170                                                         T  222
  175 NCHR=NCHR+NCNT
      REMB=OZLBL-FLOAT(IFIX(OZLBL*(10.**(NCNT+2))+0.1))/(10.**(NCNT+2))
      IF (REMB.GE.(0.001/(10.**NCNT))) NCHR=NCHR+1
      CALL CURVE (U,V,K,1,KALCMP,0,0,SX)
  185 CONTINUE
      IF (KALCMP.LE.0) GO TO 220
      CALL FRAME (0.,0.,0.,HC,HCC,HCX,HCM,IDIG1,0.,XN,XNC,XNX,XNM,IDIG2,
     19HNMHC,PPMC,9,7HNOX,PPM,7,1H ,1,1H ,1)
      NCNT=0
      DO 190 I=1,18
      IF (ITTL(I).NE.4H    ) GO TO 195
      NCNT=NCNT+1
  190 CONTINUE
  195 NLST=18-NCNT
      DO 200 I=1,NLST
  200 ITTL1(I)=ITTL(I+NCNT)
      NCNT1=18
      DO 205 I=1,18
      II=19-I
      IF (ITTL1(II).NE.4H    ) GO TO 210
      NCNT1=NCNT1-1
  205 CONTINUE
  210 NCNT1=NCNT1-NCNT
      ORGX=((HCC*HC)-(FLOAT(NCNT1)*4.*CHRZ))/2.0
      DO 215 I=1,NCNT1
      CALL SYMBOL (ORGX,ORGY,CHRZ,ITTL1(I),0.,4)
      ORGX=ORGX+4.0*CHRZ
  215 CONTINUE
      CALL PLOT (10.,2.,999)
  220 HCS=FLOAT(NW)
      XNS=FLOAT(NLL)
C 155 CALL LINPRT
      CALL LINPRT (HC,XN)
      RETURN
      END
```

## Subroutine CURVE

```
      SUBROUTINE CURVE (XARRAY,YARRAY,NPTS,INC,KALCMP,LINTYP,INTEQ,SIGMA
     1)
C
C     *** PURPOSE -- PLOTS A SMOOTH CURVE THROUGH THE DATA VALUES FROM T
C         GW LUNDBERG/SAI   JULY 177
C
C          MODIFIED BY H HOGO AUG 1977
C
C         XARRAY  ARRAY CONTAINING X VALUES
C         YARRAY  ARRAY CONTIANING Y VALUES
C         NPTS    NUMBER OF DATA POINTS IN THE ARRAYS ACTUALLY USED
C                ) 0  SCALING AT TOP OF ARRAYS
C         INC     EVERY INC POINT WILL BE USED
C         LINTYP  PLOT SPECIAL SYMBOL EVERY LINTYP POINT
C                ) 0  CONNECTED SYMBOL PLOT
C                = 0  LINE PLOT
C                ( 0  UNCONNECTED SYMBOL PLOT
C         INTEQ   INTEGER EQUIVALENT OF SPECIAL SYMBOL
C         THIS ROUTINE CALLS  SYMBOL, PLOT, KURV1 AND KURV2
C
      COMMON /VVLBL/ FCTR,DIST,CHRSZ,NCHR,OZLBL
      DIMENSION XARRAY(1), YARRAY(1), XI(50), YI(50), XP(50), YP(50), TE
     1MP(50)
C
      DATA NSLOPE/0/,SLOPE1,SLOPEN/0.,0./
C
C
C     *** LOCATE SCALING (FIRSTV AND DELTAV) FOR EACH ARRAY
C         ------ ------- ------- --- ------- --- ---- -----
C
C
C     *** SCALING IN TOP OF ARRAYS -- CALCOMP STANDARD
      N=NPTS*INC+1
      FIRSTX=XARRAY(N)
      FIRSTY=YARRAY(N)
      N=N+INC
      DELTAX=XARRAY(N)
      DELTAY=YARRAY(N)
C
      NUM=IABS(NPTS)
      IF (KALCMP.LE.0) GO TO 10
C
C     *** CHECK IF SYMBOL PLOT WANTED -- LINTYP () 0
      IF (LINTYP.EQ.0) GO TO 10
C
C     *** CENTERED SYMBOL PLOT
C         -------- ------ ----
C
C     *** SCALE FIRST DATA POINT AND PLOT CENTERED SYMBOL
      X=(XARRAY(1)-FIRSTX)/DELTAX
      Y=(YARRAY(1)-FIRSTY)/DELTAY
      CALL SYMBOL (X,Y,0.1,INTEQ,0.,-1)
C
C     *** PLOT REMAINING SYMBOLS AT INCREMENTS OF MARK
      MARK=IABS(LINTYP)
      N=1
C
```

```
      DO 5 J=2,NUM
      N=N+INC
      IF (MOD(N,MARK).NE.0) GO TO 5
      X=(XARRAY(N)-FIRSTX)/DELTAX
      Y=(YARRAY(N)-FIRSTY)/DELTAY
      CALL SYMBOL (X,Y,0.1,INTEQ,0.,-1)
    5 CONTINUE
C
C     *** IF THE SYMBOLS ARE NOT TO BE CONNECTED, RETURN
      IF (LINTYP.LT.0) GO TO 30
C
C     *** LINE PLOT (OR CONNECT SYMBOLS)
C         ---- ---- -- ------- --------
C
C     *** SCALE FIRST DATA POINT AND MOVE PEN THERE
   10 XI(1)=(XARRAY(1)-FIRSTX)/DELTAX
      YI(1)=(YARRAY(1)-FIRSTY)/DELTAY
C
C
C     *** SCALE THE REMAINING POINTS
      N=1
      DO 15 J=2,NUM
      N=N+INC
      XI(J)=(XARRAY(N)-FIRSTX)/DELTAX
      YI(J)=(YARRAY(N)-FIRSTY)/DELTAY
   15 CONTINUE
C
      NSLP=NSLOPE
C
C     *** CHECK IF PERIODIC
      IF (ABS(XI(NUM)-XI(1)).LT.0.01.AND.ABS(YI(NUM)-YI(1)).LT.0.01) NSL
     1P=-1
C
C     *** SET UP SPLINE INTERPOLATION
      NSLP=1
      SLOPE1=57.29578*ATAN((YI(1)-YI(2))/(XI(1)-XI(2)))
      IF (SLOPE1.GT.0.) SLOPE1=SLOPE1-180.
      SLOPE1=AMIN1(SLOPE1,-90.)
      SLOPEN=28.64789*ATAN((YI(N)-YI(N-1))/(XI(N)-XI(N-1)))
      CALL KURV1 (NUM,XI,YI,NSLP,SLOPE1,SLOPEN,XP,YP,TEMP,S,SIGMA)
      CALL KURV2 (0.,X,Y,NUM,XI,YI,XP,YP,S,SIGMA)
      X=AMAX1(0.,X)
      Y=AMAX1(0.,Y)
      USX=X*DELTAX+FIRSTX
      USY=Y*DELTAY+FIRSTY
      CALL SAVLIN (USX,USY)
C
C     *** LINE SEGMENTS WILL BE A TENTH INCH LONG -- S IS THE ARCLENGTH
      NP=10.*S+1
      CONST=1./NP
      DIST=S
      IF (KALCMP.LE.0) GO TO 20
      CALL VVLBLF (XI(1),YI(1))
C
C     *** MAP AND PLOT SEGMENTS
   20 DO 25 J=1,NP
      T=-J*CONST
      CALL KURV2 (T,X,Y,NUM,XI,YI,XP,YP,S,SIGMA)
      X=AMAX1(0.,X)
      Y=AMAX1(0.,Y)
      USX=X*DELTAX+FIRSTX
      USY=Y*DELTAY+FIRSTY
      CALL SAVLIN (USX,USY)
      IF (KALCMP.LE.0) GO TO 25
      CALL VVLBLC (X,Y)
   25 CONTINUE
      IF (KALCMP.LE.0) GO TO 30
      CALL VVLBLL (0.,0.)
C
   30 RETURN
C
      END
```

## Subroutine ISOPLT

```
      SUBROUTINE ISOPLT (SAVHC,SAVNOX)
      COMMON /NEED/ HC,XN,NL,NRTO,RTO(20),OZZ(20),OZN(8,20),RHO(8,20),HR
     1,OC(4),OS(2),HCS,XNS,LS,HCLL(8)
      COMMON /TITL/ ITTL(18)
      COMMON /INOUT/ IN,IOUT,ITAPE
      COMMON /CALC/ NR,KR(77,3),A(77),S(77),R(77),ITYPE(77),IA(34),JA(21
     18),DILUT,TEMP,ERR,START,STOPP,SPECIS(34),TPRN,TSTP
      COMMON /CNTRL/ SIG,SIGMA,INFO,NPTO,XNF,RCTY,ALDX,OZIN,OZAL,HCIN,HC
     1AL,XNIN,XNAL,TSRT,DTIM,Z1,Z2,DCON,EHC,EXN,FLST,TLST
      COMMON /GEAR6/ DUM1(880),OZP(20),DUM2(306),NGRID(101,2),DUM3(92)
      COMMON /HOUR/ OZM,NGO,TM
      DIMENSION TVERT(52,2), JGRID(101,42), TPRINT(11), NLINE(3)
      DIMENSION CVERT(9),TV(7),SAVDAT(101),TV1(7)
      DATA JBLANK/4H    /,MAXHC/101/,MAXNOX/42/,MAXPNT/80/,TGRID/100./,C
     1GRID/42./,JPLUS/1H+/,JBAR/1HI/,JSYMB/1H+/
      DATA CVERT /4H O  ,4H Z  ,4H O  ,4H N  ,4H E  ,4H    ,4H P  ,4H P
     1 ,4H M  /
      DATA TV/4H N  ,4H O  ,4H X  ,4H    ,4H P  ,4H P  ,4H M  /
      DATA TVERT/104*4H    /,NGRID(1,1)/1HI/,NGRID(1,2)/1HI/,NGRID(101,1
     1)/1HI/,NGRID(101,2)/1HI/
      DO 5 J=1,42
      JGRID(1,J)=JBAR
      JGRID(101,J)=JBAR
    5 CONTINUE
      DO 15 I=1,52
      TVERT(I,1)=4H
      IF (NPTO.EQ.0) GO TO 10
      IF (I.LT.18.OR.I.GT.26) GO TO 15
      K=I-17
      TVERT(I,1)=CVERT(K)
      GO TO 15
   10 IF (I.LT.17.OR.I.GT.23) GO TO 15
      K=I-16
      TVERT(I,1)=TV(K)
   15 CONTINUE
      DO 20 I=1,101
   20 SAVDAT(I)=0.
      DO 25 J=1,42,3
      JGRID(1,J)=JPLUS
      JGRID(101,J)=JPLUS
   25 CONTINUE
C
C
C SET NORMALIZATION FACTORS AND VERTICAL LABELS
C
      CLOW=0.
      TLOW=0.
      IF (NPTO.NE.0) GO TO 35
      CHIGH=XN
      CSPAN=CGRID/CHIGH
      THIGH=HC
      DO 30 I=1,7
      M=8-I
      TV1(I)=(FLOAT(M)/7.)*CHIGH
   30 CONTINUE
      GO TO 40
C
```

```
C SET HORIZONTAL LABELS
C
   35 THIGH=STOPP
   40 TSPAN=TGRID/THIGH
      DO 45 J=1,11
      TPRINT(J)=(FLOAT(J-1)/10.)*THIGH
   45 CONTINUE
C
C CLEAR GRID
C
      MAXHC1=MAXHC-1
      DO 50 K=1,MAXNOX
      DO 50 J=2,MAXHC1
      JGRID(J,K)=JBLANK
      IF (K.LE.2) NGRID(J,K)=JBLANK
   50 CONTINUE
      RETURN
C
C ENTRY FOR SAVING INTERPOLATED POINTS
C
C     ENTRY SAVLIN
      ENTRY SAVLIN (SAVHC,SAVNOX)
      KHC=IFIX((SAVHC-TLOW)*TSPAN+1.5)
      IF (NPTO.NE.0) GO TO 55
      KNOX=IFIX((SAVNOX-CLOW)*CSPAN-0.5)
      KNOX=MAXNOX-KNOX
      IF (KNOX.LT.1) GO TO 60
      IF (KNOX.GT.MAXNOX) GO TO 60
   55 IF (KHC.LT.2) GO TO 60
      IF (KHC.GT.MAXHC1) GO TO 60
      IF (NPTO.EQ.0) JGRID(KHC,KNOX)=JSYMB
      IF (NPTO.NE.0) SAVDAT(KHC)=SAVNOX
   60 RETURN
C
C ENTRY FOR PLOTTING GRID
C
C     ENTRY LINPRT
      ENTRY LINPRT (SAVHC,SAVNOX)
      IF (NPTO.NE.0) GO TO 95
      NPL=IFIX(HCS+0.1)
      NLL=IFIX(XNS+0.5)
      KOUNT=0
      IF (NLL.EQ.0) GO TO 80
      NJ=1
   65 NJ=NJ+1
      J=MAXNOX-NJ
      IF (JGRID(3,J):EQ.JBLANK) GO TO 65
      KOUNT=KOUNT+1
      IF (KOUNT.GT.NLL) GO TO 75
      IF (NJ.GT.MAXNOX-1) GO TO 75
      NVAR=IFIX(OZP(KOUNT)*100.+0.5)
      CALL CONVT (NVAR,NLINE)
      DO 70 II=1,3
   70 IF (NLINE(II).NE.1H ) JGRID(2+II,J)=NLINE(II)
      NJ=NJ+1
      GO TO 65
   75 KOUNT=KOUNT-1
   80 I=1                                                                V   113
   85 I=I+1                                                              V   114
      IF (I.GT.MAXHC1) GO TO 110                                         V   115
      IF (JGRID(I,1).EQ.JBLANK) GO TO 85                                 V   116
      KOUNT=KOUNT+1                                                      V   117
      IF (KOUNT.GT.NPL) GO TO 110                                        V   118
      NVAR=IFIX(OZP(KOUNT)*100.+0.5)                                     V   119
      CALL CONVT (NVAR,NLINE)                                            V   120
      DO 90 II=2,3                                                       V   121
   90 IF (NLINE(II).NE.1H ) NGRID(I,II-1)=NLINE(II)                      V   122
      I=I+1                                                              V   124
      GO TO 85                                                           V   125
   95 CHIGH=OZM+(0.2*OZM)                                                V   126
      IF (OZM.EQ.0.0) RETURN                                             V   126A
      CSPAN=CGRID/CHIGH                                                  V   127
      DO 100 I=1,7                                                       V   128
      M=8-I                                                              V   129
      TV1(I)=(FLOAT(M)/7.)*CHIGH                                         V   130
  100 CONTINUE                                                           V   132
      DO 105 I=2,100                                                     V   133
      IF (SAVDAT(I).EQ.0.) GO TO 105                                     V   134
      KNOX=IFIX(SAVDAT(I)*CSPAN-0.5)                                     V   135
      KNOX=MAXNOX-KNOX                                                   V   136
      IF (KNOX.LT.1) GO TO 105                                           V   137
      IF (KNOX.GT.MAXNOX) GO TO 105                                      V   138
      JGRID(I,KNOX)=1HO                                                  V   139
  105 CONTINUE                                                           V   140
  110 IF (NPTO.EQ.0) WRITE (IOUT,125) ((NGRID(I,J),I=1,101),J=1,2)       V   141
      IF (NPTO.NE.0) WRITE (IOUT,120) TVERT(1,1),TVERT(1,2)              V   142
      IF (NPTO.EQ.0) KFRST=1                                             V   143
      IF (NPTO.NE.0) KFRST=2                                             V   144
      DO 115 K=KFRST,MAXNOX                                              V   145
      L=MOD((K-1),6)                                                     V   146
      I=(K-1)/6+1                                                        V   147
      IF (L.EQ.0) WRITE (IOUT,130) TVERT(K,1),TV1(I),(JGRID(J,K),J=1,MAX V   148
     1HC)                                                                V   149
      IF (L.NE.0) WRITE (IOUT,135) TVERT(K,1),(JGRID(J,K),J=1,MAXHC)     V   150
  115 CONTINUE                                                           V   151
      WRITE (IOUT,140) CLOW                                              V   152
      IF (NPTO.EQ.0) WRITE (IOUT,145) TPRINT                             V   153
      IF (NPTO.NE.0) WRITE (IOUT,155) TPRINT                             V   154
      WRITE (IOUT,150) (ITTL(I),I=1,18)                                  V   155
      IF (NPTO.EQ.0) WRITE (IOUT,160) (OZP(I),I=1,NPL)                   V   155A
      RETURN                                                             V   156
C                                                                        V   157
C                                                                        V   158
C                                                                        V   159
  120 FORMAT (1H1,//////////,9X,A4,F5.3,1H+,10(10H---------+))           V   160
  125 FORMAT (1H1,//////,18X,1H+,10(10H---------+),/,18X,101A1,/,18X,    V   161
     1101A1)                                                             V   162
  130 FORMAT (9X,A4,F5.3,101A1)                                          V   163
  135 FORMAT (9X,A4,5X,101A1)                                            V   164
  140 FORMAT (13X,F5.3,1H+,10(10H---------+))                            V   165
  145 FORMAT (F21.3,10F10.2,/,64X,11HNMHC (PPMC),//)                     V   166
  150 FORMAT (46X,18A4)                                                  V   167
  155 FORMAT (F21.1,10F10.1,/,63X,14HTIME (MINUTES),//)                  V   168
  160 FORMAT (1H0,/,20X,20HTHE OZONE LINES ARE  ,10F8.5,/,40X,10F8.5)    V   168A
      END                                                                V   169-
```

## Subroutine CURV1

```
      SUBROUTINE CURV1 (N,X,Y,SLP1,SLPN,YP,TEMP,SIGMA)
C
C   THIS SUBROUTINE DETERMINES THE PARAMETERS NECESSARY TO
C   COMPUTE AN INTERPOLATORY SPLINE UNDER TENSION THROUGH
C   A SEQUENCE OF FUNCTIONAL VALUES.  THE SLOPES AT THE TWO
C   ENDS OF THE CURVE MAY BE SPECIFIED OR OMITTED.  FOR ACTUAL
C   COMPUTATION OF POINTS ON THE CURVE IT IS NECESSARY TO CALL
C   THE FUNCTION CURV2.
C
C   ON INPUT --
C   N = THE NUMBER OF VALUES TO BE INTERPOLATED (N.GE.2),
C   X = AN ARRAY OF THE N INCREASING ABCISSAE OF THE
C       FUNCTIONAL VALUES,
C   Y = AN ARRAY OF THE N ORDINATES OF THE VALUES, (I.E.Y(K)
C       IS THE FUNCTIONAL VALUE CORRESPONDING TO X(K)),
C   SLP1,SLPN CONTAIN THE DESIRED VALUES FOR THE FIRST
C       DERIVATIVE TO THE CURVE AT X(1) AND X(N), RESPECTIVELY,
C       IF THE QUANTITY SIGMA IS NEGATIVE THESE VALUES WILL BE
C       DETERMINED INTERNALLY AND THE USER NEED ONLY FURNISH
C       PLACE-HOLDING PARAMETERS FOR SLP1 AND SLPN.  SUCH PLACE-
C       HOLDING PARAMETERS WILL BE IGNORED BY NOT DESTROYED,
C   YP = AN ARRAY OF LENGTH AT LEAST N
C   TEMP = AN ARRAY OF LENGTH AT LEAST N WHICH IS USED FOR
C       SCRATCH STORAGE,
C   SIGMA = THE TENSION FACTOR.  THIS IS NON-ZERO AND
C       INDICATES THE CURVINESS DESIRED. IF ABS(SIGMA) IS NEARLY
C       ZERO (E.G. .001) THE RESULTING CURVE IS APPROXIMATELY A
C       CUBIC SPLINE.  IF ABS(SIGMA) IS LARGE (E.G. 50.) THE
C       RESULTING CURVE IS NEARLY A POLYGONAL LINE.  THE SIGN
C       OF SIGMA INDICATES WHETHER THE DERIVATIVE INFORMATION
C       HAS BEEN INPUT OR NOT.  IF SIGMA IS NEGATIVE THE ENDPOINT
C       DERIVATIVES WILL BE DETERMINED INTERNALLY.  A STANDARD
C       VALUE FOR SIGMA IS APPROXIMATELY 1. IN ABSOLUTE VALUE
C
C   ON OUTPUT --
C   YP = VALUES PROPORTIONAL TO THE SECOND DERIVATIVE
C       OF THE CURVE AT THE GIVEN NODES.
C   N,X,Y,SLP1 AND SIGMA ARE UNALTERED,
C
C     *** AK CLINE/NCAR, COMM. ACM 17,4(APR.1974), 221.
C
      DIMENSION X(N), Y(N), YP(N), TEMP(N)
      DATA EXPMAX/87.4/
C
      NCYC=0
      NCHG=0
      NM1=N-1
      NP1=N+1
      DELX1=X(2)-X(1)
      IF (ABS(DELX1/X(2)).LT.0.02) GO TO 55
      DX1=(Y(2)-Y(1))/DELX1
C
C     *** DETERMINE SLOPES IF NECESSARY
      IF (SIGMA.LT.0.) GO TO 45
      SLPP1=SLP1
      SLPPN=SLPN
C
```

```
C     *** DENORMALIZE TENSION FACTOR
    5 IF (ABS(X(N)-X(1))/X(N).LT.0.02) GO TO 55
      SIGMAP=ABS(SIGMA)*FLOAT(N-1)/(X(N)-X(1))
      DX1=(Y(2)-Y(1))/DELX1
C
C     *** SET UP RIGHT HAND SIDE OF TRIDIAGONAL SYSTEM
C         FOR YP AND PERFORM FORWARD ELIMINATION
      DELS=SIGMAP*DELX1
      IF (DELS.GE.EXPMAX) GO TO 55
      EXPS=EXP(DELS)
      SINHS=0.5*(EXPS-1./EXPS)
      SINHIN=1./(DELX1*SINHS)
      DIAG1=SINHIN*(DELS*0.5*(EXPS+1./EXPS)-SINHS)
      DIAGIN=1./DIAG1
      YP(1)=DIAGIN*(DX1-SLPP1)
      SPDIAG=SINHIN*(SINHS-DELS)
      TEMP(1)=DIAGIN*SPDIAG
      IF (N.EQ.2) GO TO 15
      DO 10 I=2,NM1
      DELX2=X(I+1)-X(I)
      IF (ABS(DELX2)/X(I+1).LT.0.02) GO TO 55
      DX2=(Y(I+1)-Y(I))/DELX2
      DELS=SIGMAP*DELX2
      IF (DELS.GE.EXPMAX) GO TO 55
      EXPS=EXP(DELS)
      SINHS=.5*(EXPS-1./EXPS)
      SINHIN=1./(DELX2*SINHS)
      DIAG2=SINHIN*(DELS*(.5*(EXPS+1./EXPS))-SINHS)
      DIAGIN=1./(DIAG1+DIAG2-SPDIAG*TEMP(I-1))
      YP(I)=DIAGIN*(DX2-DX1-SPDIAG*YP(I-1))
      SPDIAG=SINHIN*(SINHS-DELS)
      TEMP(I)=DIAGIN*SPDIAG
      DX1=DX2
      DIAG1=DIAG2
   10 CONTINUE
   15 DIAGIN=1./(DIAG1-SPDIAG*TEMP(NM1))
      YP(N)=DIAGIN*(SLPPN-DX2-SPDIAG*YP(NM1))
C
C     ***  PERFORM BACK SUBSTITUTION
      DO 20 I=2,N
      IBAK=NP1-I
      YP(IBAK)=YP(IBAK)-TEMP(IBAK)*YP(IBAK+1)
   20 CONTINUE
      IF (SIGMA.GT.0.) RETURN
      IF (N.EQ.3) RETURN
      IF (NCYC.GT.15) RETURN
      IF (NCYC.GT.0) GO TO 25
      XTEST=(X(3)+X(2))/2.
      YCORD=(Y(3)+Y(2))/2.
      FACT=SQRT(ABS(SIGMA))
      YTEST=(YCORD*FACT+CIRC(XTEST,X(1),Y(1))+CIRC(XTEST,X(2),Y(2)))/(2.
     1+FACT)
      DY2=CURV2(XTEST,N,X,Y,YP,SIGMA,1)-YTEST
      DSAV=DY2
      SN=-1.
      IF (DY2.GT.0.) SN=1.
      FACT=0.3*(SN+2.)
      DY2=0.
      IT=1
   25 NCYC=NCYC+1
      DY1=DY2
      DY2=CURV2(XTEST,N,X,Y,YP,SIGMA,IT)-YTEST
      IF (NCYC.GT.15) RETURN
      IF (NCYC.GT.13.AND.NCHG.LT.2) GO TO 40
      IF (SIGN(1.,DY1).NE.SIGN(1.,DY2)) GO TO 30
      IF (ABS(DY2).LT.ABS(DY1)) GO TO 35
   30 SN=-SN
      NCHG=NCHG+1
      FACT=SN*((1./(1.-SN*FACT))**(1./3.)-1.)
   35 SLPP1=SLPP1*(1.+SN*FACT)
      GO TO 5
C
   40 IF (DY2/DSAV.LT.0.2) GO TO 35
      SLPP1=SLPPX
      NCYC=15
      GO TO 5
   45 IF (N.EQ.2) GO TO 50
C
C     *** IF NO DERIVATIVES ARE GIVEN USE SECOND ORDER POLYNOMIAL
C             INTERPOLATION ON INPUT DATA FOR VALUES AT ENDPOINTS.
      SLPP1=(Y(2)-Y(1))/(X(2)-X(1))
      DELN=X(N)-X(NM1)
      DELNM1=X(NM1)-X(N-2)
      DELNN=X(N)-X(N-2)
      IF (ABS(DELN)/X(N).LT.0.02) GO TO 55
      IF (ABS(DELN)/X(N).LT.0.02) GO TO 55
      IF (ABS(DELNM1)/X(NM1).LT.0.02) GO TO 55
      IF (ABS(DELNN)/X(N).LT.0.02) GO TO 55
      C1=(DELNN+DELN)/DELNN/DELN
      C2=-DELNN/DELN/DELNM1
      C3=DELN/DELNN/DELNM1
      SLPPN=C3*Y(N-2)+C2*Y(NM1)+C1*Y(N)
      DX2=X(3)-X(2)
      DX31=X(3)-X(1)
      IF (ABS(DX2)/X(3).LT.0.02) GO TO 55
      IF (ABS(DX31)/X(3).LT.0.02) GO TO 55
      C1=-(DX31+DELX1)/DX31/DELX1
      C2=DX31/DELX1/DX2
      C3=-DELX1/DX31/DX2
      SLPPX=C1*Y(1)+C2*Y(2)+C3*Y(3)
      IF (Y(2).GT.Y(1)) SLPPX=AMAX1(0.,SLPPX)
      FACT2=SQRT(ABS(SIGMA))
      SLPPX=(SLPPX+FACT2*SLPP1)/(1.+FACT2)
      SLPP1=SLPPX
      IF (Y(N).GT.Y(NM1)) SLPPN=AMAX1(0.,SLPPN)
      SLPNL=(Y(N)-Y(NM1))/DELN
      SLPPN=(SLPPN+SLPNL*FACT2)/(1.+FACT2)
      SLPPN=(SLPPN-SLPNL*SIGMA)/(1.-SIGMA)
      GO TO 5
C
C     *** IF ONLY TWO POINTS AND NO DERIVATIVES ARE GIVEN, USE
C         STRAIGHT LINE FOR CURVE
C
   50 YP(1)=0.
      YP(2)=0.
      RETURN
   55 SIGMA=-50.
      RETURN
      END
```

# Function CURV2

```
      FUNCTION CURV2 (T,N,X,Y,YP,SIGMA,IT)
C
C    THIS FUNCTION INTERPOLATES A CURVE AT A GIVEN POINT
C    USING A SPLINE UNDER TENSION.  THE SUBROUTINE CURV1 SHOULD
C    BE CALLED EARLIER TO DETERMINE CERTAIN NECESSARY
C    PARAMETERS.
C
C    ON INPUT--
C    T = A REAL VALUE TO BE MAPPED ONTO THE
C        INTERPOLATING CURVE.
C    N = THE NUMBER OF POINTS WHICH WERE INTERPOLATED
C        TO DETERMINE THE CURVE,
C    X,Y = ARRAYS CONTAINING THE ORDINATES AND ABCISSAS
C        OF THE INTERPOLATED POINTS,
C    YP = AN ARRAY WITH VALUES PROPORTIONAL TO THE SECOND
C        DERIVATIVE OF THE CURVE AT THE NODES
C    SIGMA = THE TENSION FACTOR (ITS SIGN IS IGNORED)
C        IT IS AN INTEGER SWITCH.  IF IT IS NOT 1 THIS INDICATES
C        THAT THE FUNCTION HAS BEEN CALLED PREVIOUSLY (WITH N,X,
C        Y,YP, AND SIGMA UNALTERED) AND THAT THIS VALUE OF T
C        EXCEEDS THE PREVIOUS VALUE.  WITH SUCH INFORMATION THE
C        FUNCTION IS ABLE TO PERFORM THE INTERPOLATION MUCH MORE
C        RAPIDLY.  IF A USER SEEKS TO INTERPOLATE AT A SEQUENCE
C        OF POINTS, EFFICIENCY IS GAINED BY ORDERING THE VALUES
C        INCREASING AND SETTING IT TO THE INDEX OF THE CALL.
C        IF IT IS 1 THE SEARCH FOR THE INTERVAL (X(K),X(K+1))
C        CONTAINING T STARTS WITH K=1.
C        THE PARAMETERS N,X,Y,YP AND SIGMA SHOULD BE INPUT
C        UNALTERED FROM THE OUTPUT OF CURV1.
C
C    ON OUTPUT--
C    CURV2 = THE INTERPOLATED VALUE.  FOR T LESS THAN
C        X(1) CURV2 = Y(1).  FOR T GREATER THAN X(N) CURV2 = Y(N).
C
C    NONE OF THE INPUT PARAMETERS ARE ALTERED.
C
C     *** AK CLINE/NCAR, COMM. ACM 17,4(APR.1974), 221
C
      DIMENSION X(N), Y(N), YP(N)
C
      S=X(N)-X(1)
      IT=IABS(IT)
C
C     *** DENORMALIZE SIGMA
      SIGMAP=ABS(SIGMA)*FLOAT(N-1)/S
C
C     *** IF IT.NE. 1 START SEARCH WHERE PREVIOUSLY TERMINATED,
C         OTHERWISE START SEARCH FROM BEGINNING
      IF (IT.EQ.1) I1=2
C
C     *** SEARCH FOR INTERVAL
    5 DO 10 I=I1,N
      IF (X(I)-T) 10,10,15
   10 CONTINUE
      I=N
C
C     *** CHECK TO INSURE CORRECT INTERVAL
```

```
   15 IF (X(I-1).LE.T.OR.T.LE.X(1)) GO TO 20
C
C     *** RESTART SEARCH AND RESET I1
C         (INPUT (IT( WAS INCORRECT)
      I1=2
      GO TO 5
C
C     *** SET UP AND PERFORM INTERPOLATION
   20 IF (SIGMA.EQ.-50.) GO TO 25
      DEL1=T-X(I-1)
      DEL2=X(I)-T
      DELS=X(I)-X(I-1)
      EXPS1=EXP(SIGMAP*DEL1)
      SINHD1=.5*(EXPS1-1./EXPS1)
      EXPS=EXP(SIGMAP*DEL2)
      SINHD2=.5*(EXPS-1./EXPS)
      EXPS=EXPS1*EXPS
      SINHS=.5*(EXPS-1./EXPS)
      CURV2=(YP(I)*SINHD1+YP(I-1)*SINHD2)/SINHS+((Y(I)-YP(I))*DEL1+(Y(I-
     1I)-YP(I-1))*DEL2)/DELS
      IF ((ABS(Y(I)-CURV2)+ABS(Y(I-1)-CURV2)).GT.1.001*(ABS(Y(I)-Y(I-1))
     1)) IT=-IT
      I1=I
      RETURN
   25 IF (ABS(X(I)-X(I-1))/X(I).LT.0.02) I=I+1
      IF (I.GT.N) I=I-2
      CURV2=((T-X(I-1))*(Y(I)-Y(I-1))/(X(I)-X(I-1)))+Y(I-1)
      IT=1
      RETURN
      END
```

## Subroutine KURV1

```
      SUBROUTINE KURV1 (NPTS,X,Y,NSLOPE,SLOPE1,SLOPEN,XP,YP,TEMP,S,SIGMA
     1)
C
C    THIS SUBROUTINE DETERMINES THE PARAMETERS NECESSARY TO
C    COMPUTE AN SPLINE UNDER TENSION PASSING THROUGH A SEQUENCE
C    OF PAIRS (X(1),Y(1),....,X(N),Y(N)) IN THE PLANE, THE
C    SLOPES AT THE TWO ENDS OF THE CURVE MAY BE SPECIFIED OR
C    OMITTED, FOR ACTUAL COMPUTATION OF POINTS ON THE CURVE IT
C    IS NECESSARY TO CALL THE SUBROUTINE KURV2.
C
C    ON INPUT --
C    NPTS = THE NUMBER OF POINTS TO BE INTERPOLATED (N.GE.2),
C    X = AN ARRAY CONTAINING THE N X-COORDINATES OF THE
C        POINTS,
C    Y = AN ARRAY CONTAIING THE N Y-COODINATES OF THE
C        POINTS,
C    NSLOPE = A FLAG FOR ENDPOINT SLOPES.  IF ' 0, THIS IS A CLOSED
C        LOOP AND NO SLOPES ARE GIVEN.  IF = 0, THIS IS AN OPEN CURVE
C        AND NO SLOPES ARE GIVEN.  IF ) 0, BOTH ENDPOINT SLOPES ARE
C        GIVEN
C    SLOPE1,SLOPEN = THE DESIRED VALUES FOR THE SLOPE
C        OF THE CURVE AT (X(1),Y(1)) AND (X(N),Y(N)), RESPEC-
C        TIVELY.  THESE QUANTITIES ARE IN DEGREES AND MEASURED
C        COUNTER CLOCKWISE FROM THE POSITIVE X-AXIS.  THE POSITIVE
C        SENSE OF THE CURVE IS ASSUMED TO BE THAT MOVING FROM THE
C        POINT 1 TO POINT N.
C    XP,YP = ARRAYS OF LENGTH AT LEAST N,
C    TEMP = AN ARRAY OF LENGTH AT LEAST N WHICH IS USED FOR
C        SCRATCH STORAGE,
C    SIGMA = THE TENSION FACTOR.  THIS IS NON-ZERO AND
C        INDICATES THE CURVINESS DESIRED.  IF SIGMA IS VERY
C        LARGE (E.G. 50.) THE RESULTING CURVE IS VERY NEARLY A
C        POLYGONAL LINE.  A STANDARD VALUE FOR SIGMA IS 1.
C
C    ON OUTPUT -
C    N,X,Y,SLOPE1,SLOPEN, AND SIGMA ARE UNALTERED,
C    XP,YP CONTAIN INFORMATION ABOUT THE CURVATURE OF THE
C        CURVE AT THE GIVEN NODE,
C    S = THE POLYGONAL ARCLENGTH OF THE CURVE.
C
C     *** AK CLINE, COMM. ACM 17,4(APR.1974), 221
C         MODIFIED BY GW LUNDBERG/SAI  MAY :77
C
      DIMENSION X(NPTS), Y(NPTS), XP(NPTS), YP(NPTS), TEMP(NPTS)
C
      DATA EXPMAX/87.4/
      TEMAX=-9999.
      DEGRAD=3.1415926/180.
      N=NPTS
      SLP1=SLOPE1
      SLPN=SLOPEN
      NM1=N-1
      NP1=N+1
      DELX1=X(2)-X(1)
      DELY1=Y(2)-Y(1)
      DELS1=SQRT(DELX1*DELX1+DELY1*DELY1)
      DX1=DELX1/DELS1
      DY1=DELY1/DELS1
C
C      *** DETERMINE SLOPES IF NECESSARY
       IF (NSLOPE) 50,40,5
    5 SLPP1=SLP1*DEGRAD
      SLPPN=SLPN*DEGRAD
C
C     *** SET UP RIGHT HAND SIDES OF TRIDIAGONAL LINEAR SYSTEM FOR
C         XP AND YP
   10 XP(1)=DX1-COS(SLPP1)
      YP(1)=DY1-SIN(SLPP1)
      TEMP(1)=DELS1
      S=DELS1
      IF (N.EQ.2) GO TO 20
      DO 15 I=2,NM1
      DELX2=X(I+1)-X(I)
      DELY2=Y(I+1)-Y(I)
      DELS2=SQRT(DELX2*DELX2+DELY2*DELY2)
      DX2=DELX2/DELS2
      DY2=DELY2/DELS2
      XP(I)=DX2-DX1
      YP(I)=DY2-DY1
      TEMP(I)=DELS2
      TEMAX=AMAX1(TEMAX,TEMP(I))
      DELX1=DELX2
      DELY1=DELY2
      DELS1=DELS2
      DX1=DX2
      DY1=DY2
C
C     *** ACCUMULATE POLYGONAL ARCLENGTH
      S=S+DELS1
   15 CONTINUE
   20 XP(N)=COS(SLPPN)-DX1
      YP(N)=SIN(SLPPN)-DY1
C
C     *** DENORMALIZE TENSION FACTOR
      SIGMAP=ABS(SIGMA)*FLOAT(N-1)/S
      DELT1=SIGMAP*TEMAX
      IF (DELT1.LT.EXPMAX) GO TO 21
      SIGMAP=0.9*EXPMAX/TEMAX
      SGN=1.0
      IF (SIGMA.LT.0.) SGN=-1.0
      SIGMA=SIGMAP*SGN*S/FLOAT(N-1)
   21 CONTINUE
C
C     *** PERFORM FORWARD ELIMINATION ON TRIDIAGONAL SYSTEM
      DELS=SIGMAP*TEMP(1)
      EXPS=EXP(DELS)
      SINHS=.5*(EXPS-1./EXPS)
      SINHIN=1./(TEMP(1)*SINHS)
      DIAG1=SINHIN*(DELS*.5*(EXPS+1./EXPS)-SINHS)
      DIAGIN=1./DIAG1
      XP(1)=DIAGIN*XP(1)
      YP(1)=DIAGIN*YP(1)
      SPDIAG=SINHIN*(SINHS-DELS)
      TEMP(1)=DIAGIN*SPDIAG
      IF (N.EQ.2) GO TO 30
      DO 25 I=2,NM1
      DELS=SIGMAP*TEMP(I)
      EXPS=EXP(DELS)
      SINHS=.5*(EXPS-1./EXPS)
      SINHIN=1./(TEMP(I)*SINHS)
      DIAG2=SINHIN*(DELS*(.5*(EXPS+1./EXPS))-SINHS)
      DIAGIN=1./(DIAG1+DIAG2-SPDIAG*TEMP(I-1))
      XP(I)=DIAGIN*(XP(I)-SPDIAG*XP(I-1))
      YP(I)=DIAGIN*(YP(I)-SPDIAG*YP(I-1))
      SPDIAG=SINHIN*(SINHS-DELS)
      TEMP(I)=DIAGIN*SPDIAG
      DIAG1=DIAG2
   25 CONTINUE
   30 DIAGIN=1./(DIAG1-SPDIAG*TEMP(NM1))
      XP(N)=DIAGIN*(XP(N)-SPDIAG*XP(NM1))
      YP(N)=DIAGIN*(YP(N)-SPDIAG*YP(NM1))
C
C     *** PERFORM BACK SUBSTITUTION
      DO 35 I=2,N
      IBAK=NP1-I
      XP(IBAK)=XP(IBAK)-TEMP(IBAK)*XP(IBAK+1)
      YP(IBAK)=YP(IBAK)-TEMP(IBAK)*XP(IBAK+1)
   35 CONTINUE
      RETURN
   40 IF (N.EQ.2) GO TO 45
C
C     *** IF NO SLOPES ARE GIVEN, USE SECOND ORDER INTERPOLATION ON
C         INPUT DATA FOR SLOPES AT ENDPOINTS
      DELS2=SQRT((X(3)-X(2))**2+(Y(3)-Y(2))**2)
      DELS12=DELS1+DELS2
      C1=-(DELS12+DELS1)/DELS12/DELS1
      C2=DELS12/DELS1/DELS2
      C3=-DELS1/DELS12/DELS2
      SX=C1*X(1)+C2*X(2)+C3*X(3)
      SY=C1*Y(1)+C2*Y(2)+C3*Y(3)
      SLPP1=ATAN2(SY,SX)
      DELNM1=SQRT((X(N-2)-X(NM1))**2+(Y(N-2)-Y(NM1))**2)
      DELN=SQRT((X(NM1)-X(N))**2+(Y(NM1)-Y(N))**2)
      DELNN=DELNM1+DELN
      C1=(DELNN+DELN)/DELNN/DELN
      C2=-DELNN/DELN/DELNM1
      C3=DELN/DELNN/DELNM1
      SX=C3*X(N-2)+C2*X(NM1)+C1*X(N)
      SY=C3*Y(N-2)+C2*Y(NM1)+C1*Y(N)
      SLPPN=ATAN2(SY,SX)
      GO TO 10
C
C     *** IF ONLY TWO POINTS AND NO SLOPES ARE GIVEN, USE STRAIGHT
C         LINE SEGMENT FOR CURVE
   45 XP(1)=0.
      XP(2)=0.
      YP(1)=0.
      YP(2)=0.
      RETURN
C
C     *** CLOSED LOOP -- PERIODIC SPLINE -- CALCULATE SLOPES
```

```
C         FOR JOIN
   50 DELN=SQRT((X(NM1)-X(N))**2+(Y(NM1)-Y(N))**2)
      DELNN=DELS1+DELN
      C1=-DELS1/DELN/DELNN
      C2=(DELS1-DELN)/DELS1/DELN
      C3=DELN/DELNN/DELS1
      SX=C1*X(NM1)+C2*X(1)+C3*X(2)
      SY=C1*Y(NM1)+C2*Y(1)+C3*Y(2)
      IF (SX.EQ.0..AND.SY.EQ.0.) SX=1
      SLPP1=ATAN2(SY,SX)
      SLPPN=SLPP1
      GO TO 10
      END
```

## Subroutine KURV2

```
      SUBROUTINE KURV2 (T,XS,YS,N,X,Y,XP,YP,S,SIGMA)
C
C    THIS SUBROUTINE PERFORMS THE MAPPING OF POINTS IN THE
C    INTERVAL (0.,1.) ONTO A CURVE IN THE PLANE.  THE SUBROUTINE
C    KURV1 SHOULD BE CALLED EARLIER TO DETERMINE CERTAIN
C    NECESSARY PARAMETERS.  THE RESULTING CURVE HAS A PARAMETRIC
C    REPRESENTATION BOTH OF WHOSE COMPONENTS ARE SPLINES UNDER
C    TENSION AND FUNCTIONS OF THE POLYGONAL ARCLENGTH PARAMETER.
C
C    ON INPUT--
C    T = A REAL VALUE OF ABSOLUTE VALUE LESS THAN OR
C        EQUAL TO 1.  TO BE MAPPED TO A POINT ON THE CURVE.  THE
C        SIGN OF T IS IGNORED AND THE INTERVAL (0.,1.) IS MAPPED
C        ONTO THE ENTIRE CURVE.  IF T IS NEGATIVE THIS INDICATES
C        THAT THE SUBROUTINE HAS BEEN CALLED PREVIOUSLY (WITH ALL
C        OTHER INPUT VARIABLES UNALTERED) AND THAT THIS VALUE OF
C        T EXCEEDS THE PREVIOUS VALUE IN ABSOLUTE VALUE.  WITH
C        SUCH INFORMATION THE SUBROUTINE IS ABLE TO MAP THE POINT
C        MUCH MORE RAPIDLY.  THUS IF THE USER SEEKS TO MAP A
C        SEQUENCE OF POINTS ONTO THE SAME CURVE, EFFICIENCY IS
C        GAINED BY ORDERING THE VALUES INCREASING IN MAGNITUDE
C        AND SETTING THE SIGNS OF ALL BUT THE FIRST, NEGATIVE.
C    N = THE NUMBER OF POINTS WHICH WERE INTERPOLATED
C        TO DETERMINE THE CURVE.
C    X,Y = ARRAYS CONTAINING THE X- AND Y-COORDINATES
C        OF THE INTERPOLATED POINTS.
C    XP,YP = THE ARRAYS OUTPUT FROM KURV2 CONTAINING
C        CURVATURE INFORMATION.
C    S = THE POLYGONAL ARCLENGTH OF THE CURVE.
C    SIGMA = THE TENSION FACTOR (ITS SIGN IS IGNORED).
C
C    THE PARAMETERS N,X,Y,XP,UP,S, AND SIGMA SHOULD BE INPUT
C    UNALTERED FROM THE OUTPUT OF KURV1.
C
C    ON  OUTPUT--
C    XS,YS = THE X- AND Y-COORDINATES OF THE IMAGE
C        POINT ON THE CURVE.
C    T,N,X,Y,XP,YP,S, AND SIGMA ARE UNALTERED.
C
      DIMENSION X(N), Y(N), XP(N), YP(N)
C
C     *** DENORMALIZE SIGMA
      SIGMAP=ABS(SIGMA)*FLOAT(N-1)/S
C
C     *** STRETCH UNIT INTERVAL INTO ARCLENGTH DISTANCE
      TN=ABS(T*S)
C
C     *** FOR NEGATIVE T START SEARCH WHERE PREVIOUSLY TERMINATED.
C         OTHERWISE START FROM BEGINNING
      IF (T.LT.0.) GO TO 5
      I1=2
      XS=X(1)
      YS=Y(1)
      SUM=0.
      IF (T.LE.0.) RETURN
    5 CONTINUE
C
```

```
C     *** DETERMINE INTO WHICH SEGMENT TN IS MAPPED
      DO 15 I=I1,N
      DELX=X(I)-X(I-1)
      DELY=Y(I)-Y(I-1)
      DELS=SQRT(DELX*DELX+DELY*DELY)
      IF (SUM+DELS-TN) 10,20,20
   10 SUM=SUM+DELS
   15 CONTINUE
C
C     *** IF ABS(T) IS GREATER THAN 1., RETURN TERMINAL POINT ON
C         CURVE
C
      XS=X(N)
      YS=Y(N)
      RETURN
C
C     *** SET UP AND PERFORM INTERPOLATION
   20 DEL1=TN-SUM
      DEL2=DELS-DEL1
      EXPS1=EXP(SIGMAP*DEL1)
      SINHD1=.5*(EXPS1-1./EXPS1)
      EXPS=EXP(SIGMAP*DEL2)
      SINHD2=.5*(EXPS-1./EXPS)
      EXPS=EXPS1*EXPS
      SINHS=.5*(EXPS-1./EXPS)
      XS=(XP(I)*SINHD1+XP(I-1)*SINHD2)/SINHS+((X(I)-XP(I))*DEL1+(X(I-1)-
     1XP(I-1))*DEL2)/DELS
      YS=(YP(I)*SINHD1+YP(I-1)*SINHD2)/SINHS+((Y(I)-YP(I))*DEL1+(Y(I-1)-
     1YP(I-1))*DEL2)/DELS
      I1=I
      RETURN
      END
```

# Subroutine FRAME

```
      SUBROUTINE FRAME (X,Y,FRSTX,FINX,SIZX,TICX,STEPX,NDECX,FRSTY,FINY,
     1SIZY,TICY,STEPY,NDECY,LBLBOT,NB,LBLLFT,NL,LBLTOP,NT,LBLRGT,NR)
C
C     *** PURPOSE -- PREPARES AN ANNOTATED FOUR SIDED FRAME
C         WITH LOWER LEFT CORNER AT (X,Y)
C             GWL/SAI  MARCH 177
C
C         SEE SUBROUTINE AXES FOR DESCRIPTION OF ARGUMENTS
C
      COMMON /PLTVEC/ HCT(20),OT(20),NH,OHC,HCG,PLTGRD,OXN,XNG,HCC,XNC,T
     1ICZ,DIGZ,CHRZ
C
C     *** CALCULATE THE AXES LENGTHS
      XLEN=(FINX-FRSTX)*SIZX
      YLEN=(FINY-FRSTY)*SIZY
C
C     *** PLACE GRIDDED LINES ON PLOT
C
      IF (ABS(PLTGRD).EQ.0.) GO TO 40
      IF (PLTGRD.LT.0.) GO TO 25
      CALL NEWPEN (2)
      STINC=(STEPY/10.)*SIZY
      ILP=FINY/STEPY+.005
      ILP=ILP*10-1
      STVAL=STINC
      J=1
      DO 10 I=1,ILP
      IF (J.EQ.2) GO TO 5
      CALL PLOT (X,STVAL,3)
      CALL PLOT (XLEN,STVAL,2)
      STVAL=STVAL+STINC
      J=2
      GO TO 10
    5 CALL PLOT (XLEN,STVAL,3)
      CALL PLOT (X,STVAL,2)
      STVAL=STVAL+STINC
      J=1
   10 CONTINUE
      STINC=(STEPX/10.)*SIZX
      ILP=FINX/STEPX+.005
      ILP=ILP*10-1
      STVAL=STINC
      J=1
      DO 20 I=1,ILP
      IF (J.EQ.2) GO TO 15
      CALL PLOT (STVAL,Y,3)
      CALL PLOT (STVAL,YLEN,2)
      STVAL=STVAL+STINC
      J=2
      GO TO 20
   15 CALL PLOT (STVAL,YLEN,3)
      CALL PLOT (STVAL,Y,2)
      STVAL=STVAL+STINC
      J=1
   20 CONTINUE
      CALL NEWPEN (1)
      GO TO 40
```

```
C
C     PLOT GRIDDED LINES WITH MATRIX PLOTTER
C
   25 IPLT=IFIX(PLTGRD)
      CALL NEWPEN (IPLT)
      STINC=(STEPY/10.)*SIZY
      ILP=IFIX(FINY/STEPY+0.005)*10-1
      STVAL=STINC
      DO 30 I=1,ILP
      IF (MOD(I,10).EQ.0) CALL NEWPEN (IPLT+1)
      CALL PLOT (X+0.01,STVAL,3)
      CALL PLOT (XLEN,STVAL,2)
      IF (MOD(I,10).EQ.0) CALL NEWPEN (IPLT)
      STVAL=STVAL+STINC
   30 CONTINUE
      STINC=(STEPX/10.)*SIZX
      ILP=IFIX(FINX/STEPX+0.005)*10-1
      STVAL=STINC
      DO 35 I=1,ILP
      IF (MOD(I,10).EQ.0) CALL NEWPEN (IPLT+1)
      CALL PLOT (STVAL,Y-0.02,3)
      CALL PLOT (STVAL,Y,3)
      CALL PLOT (STVAL,YLEN,2)
      IF (MOD(I,10).EQ.0) CALL NEWPEN (IPLT)
      STVAL=STVAL+STINC
   35 CONTINUE
      CALL NEWPEN (0)
   40 CONTINUE
C
C     *** PLOT THE FOUR SIDES WITH ANNOTATIONS
      CALL AXES (X,Y,FRSTX,FINX,SIZX,TICX,STEPX,NDECX,0.,LBLBOT,-NB,1)
      CALL AXES (X,Y,FRSTY,FINY,SIZY,TICY,STEPY,NDECY,90.,LBLLFT,NL,1)
      CALL AXES (X,Y+YLEN,FRSTX,FINX,SIZX,TICX,STEPX,NDECX,0.,LBLTOP,NT,
     1-1)
      CALL AXES (X+XLEN,Y,FRSTY,FINY,SIZY,TICY,STEPY,NDECY,90.,LBLRGT,-N
     1R,-1)
C
      RETURN
      END
```

## Subroutine AXES

```
      SUBROUTINE AXES (X,Y,FIRSTV,FINALV,SCALE,TSTEP,ASTEP,NDEC,ANGLE,IB
     1CD,NCHAR,LABEL)
C
C     *** SAI SUBROUTINE AXES
C         GW LUNDBERG/SAI  DEC 76
C
C         X,Y = COORDINATES IN INCHES OF AXIS LINE STARTING
C               POINT
C         FIRSTV = STARTING VALUE FOR THE AXIS
C         FINALV = ENDING VALUE FOR THE AXIS
C         SCALE = INCHES/UNIT FOR FIRSTV,FINALV,TSTEP,ASTEP
C         TSTEP = STEP SIZE FOR TICS
C         ASTEP = STEP SIZE FOR LABELED TICS
C         NDEC = FORMAT FOR LABELS -- SEE SUBROUTINE NUMBER
C         ANGLE = ANGLE OF AXIS IN DEGREES FROM HORIZONTAL
C         IBCD = THE AXIS TITLE AS ARRAY OR HOLLERITH STRING
C         NCHAR = NUMBER OF CHARACTERS IN TITLE
C               ) 0, TIC MARKS, ANNOTATION AND TITLE PLOTTED ON
C                   CLOCKWISE SIDE OF AXIS LINE
C               ( 0, ON COUNTER CLOCKWISE SIDE
C
C         THIS ROUTINE WAS WRITTEN FOR A MATRIX PLOTTER -- IT DOES
C         NOT OPTIMIZE PEN MOVEMENTS.  THE ROUTINE SHOULD BE MACHINE
C         INDEPENDENT
C
C
C     *** FOLLOWING ARE ADJUSTABLE -- IF LABEL ) 0, ALL TICS ARE
C         LABELED, IF LABEL = 0, THE LAST TIC IS NOT LABELED,
C         IF LABEL ( 0, THE FIRST AND LAST ARE NOT LABELED
C
C     *** DEFINE VARIOUS CHARACTER SIZES
      COMMON /PLTVEC/ HCT(20),OT(20),NH,OHC,HCG,PLTGRD,OXN,XNC,HC1,XN1,T
     1ICSIZ,DIGSIZ,CHRSIZ
C
C     *** STEP 1 -- DRAW AXIS AND TIC MARKS
C         ---- -    ---- ---- --- --- -----
C
C     *** MOVE PEN TO START OF AXIS
      X0=X
      Y0=Y
      CALL PLOT (X0,Y0,3)
C
C     *** LOCATE THE OTHER END AND DRAW AXIS
      COSA=COS(ANGLE*0.017453294)
      SINA=SIN(ANGLE*0.017453294)
      AXLEN=(FINALV-FIRSTV)*SCALE
      X1=X0+AXLEN*COSA
      Y1=Y0+AXLEN*SINA
      CALL PLOT (X1,Y1,2)
C
C     *** ADD THE TIC MARKS ON WRONG SIDE OF AXIS
      POS=FLOAT(ISIGN(1,NCHAR))
      IF (TSTEP.EQ.0.) GO TO 10
      NTIC=(FINALV-FIRSTV)/TSTEP+1.5
      DO 5 J=1,NTIC
C
C         *** MOVE PEN TO START OF TIC
```

```
      X1=X0+FLOAT(J-1)*TSTEP*SCALE*COSA
      Y1=Y0+FLOAT(J-1)*TSTEP*SCALE*SINA
      CALL PLOT (X1,Y1,3)
C
C         *** DRAW A TIC NORMAL TO AXIS
      X1=X1+TICSIZ*POS*SINA
      Y1=Y1-TICSIZ*POS*COSA
      CALL PLOT (X1,Y1,2)
    5 CONTINUE
C
C     *** STEP 2 -- SET IN LABELED TICS ON CORRECT SIDE OF AXIS
C         ---- -    --- -- ------- ---- -- ------- ---- -- ----
C
   10 IF (ASTEP.EQ.0.) GO TO 25
      NTIC=(FINALV-FIRSTV)/ASTEP+1.5
      NFRST=1
      NLST=NTIC
      IF (LABEL.LE.0) NLST=NLST-1
      IF (LABEL.LT.0) NFRST=NFRST+1
      DO 15 J=NFRST,NLST
      X1=X0+FLOAT(J-1)*ASTEP*SCALE*COSA
      Y1=Y0+FLOAT(J-1)*ASTEP*SCALE*SINA
      CALL PLOT (X1,Y1,3)
C
      X1=X1-TICSIZ*POS*SINA
      Y1=Y1+TICSIZ*POS*COSA
      CALL PLOT (X1,Y1,2)
   15 CONTINUE
C
C     *** STEP 3 -- ANNOTATE THE TIC MARKS
C         ---- -    -------- --- --- -----
C
C     *** DETERMINE PERPENDICULAR OFFSET TO BOTTOM OF CHARACTER
      OFFSET=TICSIZ+0.03
      IF (POS.NE.1) OFFSET=OFFSET+DIGSIZ
C
C     *** CALCULATE LOCATION OF FIRST CHARACTER
      X0=X0-DIGSIZ*COSA
      Y0=Y0-DIGSIZ*SINA
      X0=X0-OFFSET*POS*SINA
      Y0=Y0+OFFSET*POS*COSA
C
C     *** ANNOTATE THE TIC MARKS
      NFRST=1
      NLAST=NTIC
      IF (LABEL.LE.0) NLAST=NLAST-1
      IF (LABEL.LT.0) NFRST=NFRST+1
      DO 20 J=NFRST,NLAST
C
C         *** GET FLOATING POINT VALUE OF ANNOTATION
      FPN=FIRSTV+FLOAT(J-1)*ASTEP
C
C         *** GET LOCATION AND PLOT FPN
      X1=X0+FLOAT(J-1)*ASTEP*SCALE*COSA
      Y1=Y0+FLOAT(J-1)*ASTEP*SCALE*SINA
      CALL NUMBER (X1,Y1,DIGSIZ,FPN,ANGLE,NDEC)
   20 CONTINUE
```

```
C
C     *** STEP 4 -- ADD AXIS TITLE
C         ---- -    --- ---- -----
C
   25 IF (NCHAR.EQ.0) GO TO 30
C     *** SET TITLE OFFSET -- DISTANCE FROM AXIS TO CHARACTERS
      OFFSET=TICSIZ+DIGSIZ+0.10
      IF (NCHAR.LT.0) OFFSET=OFFSET+CHRSIZ
C
C     *** CALCULATE TITLE SIZE
      TSIZ=CHRSIZ*IABS(NCHAR)
C
C     *** CALCULATE OFFSET FROM BEGINNING OF AXIS TO FIRST CHARACTER
      OFF=0.5*(AXLEN-TSIZ)
C
C     *** CALCULATE LOCATION OF FIRST CHARACTER AND PLOT TITLE
      X0=X+OFF*COSA
      Y0=Y+OFF*SINA
      X0=X0-OFFSET*POS*SINA
      Y0=Y0+OFFSET*POS*COSA
      CALL SYMBOL (X0,Y0,CHRSIZ,IBCD,ANGLE,IABS(NCHAR))
C
C         FINISHED
   30 RETURN
      END
```

# Block Data SUN

```
 BLOCK DATA SUN
 COMMON /SUNLIT/ XJ(47,10),SIGMA(31,10),PHI(31,10),Z(10),RTCON(10),
1LAM1,INC,SLA,SLO,TZ,IY,IM,ID,ISTRT,ISTOP,IINC,IEND,SPECIE,MAXZ,ITI
2ME(015),XZ(015),K(015),JSTRT,JSTOP,SPEC(11),MNLM(11),MXLM(11),MAXL
3,MAXJ
 COMMON /PHOTON/ CF(45,8),P(15,9),IPH(9)
 DATA IPH/1,12,19,18,50,49,17,53,0/
 DATA MAXL,MAXZ,MAXJ,LAM1,INC/09,10,47,2900,100/
 DATA (Z(I),I=1,10)/0.,10.,20.,30.,40.,50.,60.,70.,78.,86./
 DATA (XJ(1,J),J=1,10)/0.00015,0.00015,8*0.0/
 DATA (XJ(2,J),J=1,10)/.039835,.038015,0.032546,.024647,.0155188,.0
1074586,.002285,.0003046,2*0.0/
 DATA (XJ(3,J),J=1,10)/.4394,.4313000,.4012000,.3505500,.2814000,.1
1978000,.1104300,.039249,.009269,.0009416/
 DATA (XJ(4,J),J=1,10)/.9551,.9438000,.9006000,.8261000,.7174000,.5
1706000,.3890000,.19372,.06372,.008893/
 DATA (XJ(5,J),J=1,10)/1.6132,1.5944000,1.5384000,1.4402000,1.29220
100,1.0832000,.8031000,.4628,.20291,.03894/
 DATA (XJ(6,J),J=1,10)/1.7134,1.6964000,1.6450000,1.5547000,1.41600
100,1.2153000,.9357000,.5726,.2689,.06149/
 DATA (XJ(7,J),J=1,10)/1.8924,1.8748000,1.8237000,1.7327000,1.59150
100,1.3834000,1.2429000,.6841,.3276,.07653/
 DATA (XJ(8,J),J=1,10)/1.9508,1.9335000,1.8849000,1.7982000,1.66210
100,1.4590000,1.1638000,.7493,.3626,.08341/
 DATA (XJ(9,J),J=1,10)/2.3974,2.3782000,2.3233000,2.2238000,2.06680
100,1.8310000,1.4799000,.9722,.4767,.10653/
 DATA (XJ(10,J),J=1,10)/2.3177,2.3008000,2.2508000,2.1609000,2.0189
1000,1.8026000,1.4751000,.9879,.4913,.1065/
 DATA (XJ(11,J),J=1,10)/2.3415,2.3254000,2.2789000,2.1947000,2.0594
1000,1.8520000,1.5336000,1.0468,.5291,.11136/
 DATA (XJ(12,J),J=1,10)/3.1737,3.1530000,3.0929000,2.9841000,2.8100
1000,2.5412000,2.1246000,1.4744,.758,.15557/
 DATA (XJ(13,J),J=1,10)/3.9935,3.9685000,3.8957000,3.7652000,3.5559
1000,3.2319000,2.7246000,1.9188,1.0035,.20173/
 DATA (XJ(14,J),J=1,10)/4.1188,4.0949000,4.0250000,3.8985000,3.6956
1000,3.3780000,2.8754000,2.0589,1.0973,.21538/
 DATA (XJ(15,J),J=1,10)/4.22245,4.1180000,4.0509500,3.9301500,3.734
18000,3.4279500,2.9379000,2.12855,1.15135,.222625/
 DATA (XJ(16,J),J=1,10)/4.6172,4.5120000,4.4421000,4.3168499,4.1135
1000,3.7932000,3.2742000,2.40225,1.3207,.250665/
 DATA (XJ(17,J),J=1,10)/5.2089,5.1817000,5.1007500,4.9576500,4.7279
1500,4.3661000,3.7832500,2.79965,1.55895,.292135/
 DATA (XJ(18,J),J=1,10)/5.6146,5.5851500,5.4983500,5.3444500,5.0991
1000,4.7150000,4.0991000,3.05525,1.72055,.318835/
 DATA (XJ(19,J),J=1,10)/5.7505,5.7211000,5.6363000,5.4851000,5.2420
1000,4.8484500,4.2483000,3.19345,1.82055,.333/
 DATA (XJ(20,J),J=1,10)/5.7988,5.7708000,5.6876500,5.5407500,5.3036
1000,4.9180000,4.3271000,3.2775,1.88745,.3398/
 DATA (XJ(21,J),J=1,10)/5.78355,5.7564500,5.6759000,5.5333000,5.304
16500,4.9435500,4.3521500,3.3168,1.9265,.3416/
 DATA (XJ(22,J),J=1,10)/5.8866,5.8571500,5.7735000,5.6254000,5.3897
1000,5.0215500,4.4222500,3.3773,1.97045,.34205/
 DATA (XJ(23,J),J=1,10)/5.93495,5.9050500,5.8182500,5.6660000,5.424
17000,5.0527000,4.4501500,3.405,1.99415,.3394/
 DATA (XJ(24,J),J=1,10)/5.9353,5.9032000,5.8178500,5.6686000,5.4327
1000,5.0667000,4.4724000,3.43375,2.0198,.3376/
 DATA (XJ(25,J),J=1,10)/5.9797,5.9503500,5.8656000,5.7171000,5.4816
```

```
1500,5.1156000,4.5209500,3.4756,2.0455,0.33125/
 DATA (XJ(26,J),J=1,10)/5.92715,5.8988000,5.8161500,5.6701500,5.439
12500,5.0801500,4.4947500,3.46155,2.03995,0.3217/
 DATA (XJ(27,J),J=1,10)/5.90955,5.8814500,5.7972500,5.6504500,5.419
17000,5.0612000,4.4787000,3.4521,2.03715,0.3147/
 DATA (XJ(28,J),J=1,10)/5.96875,5.9396500,5.8528500,5.7025500,5.467
11000,5.1035000,4.5142000,3.47855,2.05155,0.30865/
 DATA (XJ(29,J),J=1,10)/6.0576,6.0280000,5.9412000,5.7889500,5.5507
1000,5.1827500,4.5650500,3.53355,2.0813,0.30345/
 DATA (XJ(30,J),J=1,10)/6.1739,6.1445000,6.0576000,5.9047000,5.6665
1000,5.2964000,4.7142000,3.6287,2.1482,0.3108/
 DATA (XJ(31,J),J=1,10)/6.2265,6.1975000,6.1110000,5.9585000,5.7225
1000,5.3540000,4.7538500,3.6857,2.1941,0.3201/
 DATA (XJ(32,J),J=1,10)/6.26925,6.2397500,6.1517500,5.9972500,5.757
17500,5.3875000,4.7846750,3.714,2.2163,0.323675/
 DATA (XJ(33,J),J=1,10)/6.312,6.2820000,6.1925000,6.0360000,5.79300
100,5.4210000,4.8155000,3.7423,2.2425,0.32725/
 DATA (XJ(34,J),J=1,10)/6.321,6.2917500,6.2047500,5.9370000,5.63775
100,5.4517500,4.6578000,3.79835,2.30265,0.34945/
 DATA (XJ(35,J),J=1,10)/6.33,6.3015000,6.2170000,5.8380000,5.482500
10.5.4825000,4.9001000,3.8544.2.3628,0.37165/
 DATA (XJ(36,J),J=1,10)/6.4215.6.3922500,6.3060000,6.0392500,5.7432
1500,5.5620000,4.9790500,3.93455,2.437625,0.400375/
 DATA (XJ(37,J),J=1,10)/6.513,6.4830000,6.3950000,6.2405000,6.00400
100,5.6415000,5.0580000,4.0147,2.51245,0.4291/
 DATA (XJ(38,J),J=1,10)/6.59375,6.5630000,6.4720000,6.3142500,6.074
16000,5.7082500,5.1225000,4.078575,2.5737,0.454825/
 DATA (XJ(39,J),J=1,10)/6.6745.6.6430000,6.5490000,6.3880000,6.1440
1000,5.7750000,5.1870000,4.14245,2.63495,0.48055/
 DATA (XJ(40,J),J=1,10)/6.659,6.6265000,6.5367500,6.3787500,6.13925
100,5.7772500,5.1992500,4.167625,2.670625,0.49945/
 DATA (XJ(41,J),J=1,10)/6.6435,6.6100000,6.5245000,6.3695000,6.1345
1000,5.7795000,5.2115000,4.1928,2.7063,0.5184/
 DATA (XJ(42,J),J=1,10)/6.46,6.45,6.35,6.20,5.98,5.71,5.15,4.09,2.7
14.0.53/
 DATA (XJ(43,J),J=1,10)/6.40,6.38,6.29,6.14,5.91,5.65,5.11,4.07,2.7
15,0.54/
 DATA (XJ(44,J),J=1,10)/6.34,6.32,6.22,6.08,5.87,5.60,5.05,4.05,2.7
16,0.56/
 DATA (XJ(45,J),J=1,10)/6.27,6.25,6.16,6.02,5.80,5.55,5.02,4.04,2.7
17,0.56/
 DATA (XJ(46,J),J=1,10)/6.21,6.19,6.10,5.96,5.75,5.49,4.97,4.02,2.7
18,0.58/
 DATA (XJ(47,J),J=1,10)/6.14,6.12,6.03,5.90,5.68,5.43,4.92,4.00,2.7
19,0.59/
 DATA SPEC/4H NO2,4HHONO,4HO33P,4HO31D,4HFOR1,4HFOR2,4HH2O2,4HALD2,
14HO3CH,4H    ,4H    /
 DATA MNLM/8*2900,4500,0,0/
 DATA MXLM/4500,3900,3500,3100,3600,3600,3700,3400,7500,0,0/
 DATA (SIGMA(I,1),I=1,17)/8.52E-20,1.28E-19,1.83E-19,2.47E-19,3.10E
1-19,3.74E-19,4.49E-19,5.01E-19,5.41E-19,5.70E-19,5.82E-19,5.95E-19
2,5.80E-19,5.45E-19,5.15E-19,4.85E-19,4.55E-19/
 DATA (PHI(J,1),J=1,17)/0.988,0.980,0.972,0.964,0.956,0.948,0.940,0
1.932,0.924,0.916,0.903,0.699,0.175,0.025,0.006,0.001,0.000/
 DATA (SIGMA(I,2),I=1,12)/0.79E-20,0.79E-20,1.14E-20,1.75E-20,2.86E
1-20,4.23E-20,5.29E-20,3.98E-20,6.08E-20,3.33E-20,1.78E-20,0.0/
 DATA (PHI(J,2),J=1,12)/0.0,9*1.0,2*0.0/
 DATA (SIGMA(I,3),I=1,07)/1.62E-18,4.44E-19,1.19E-19,3.36E-20,8.79E
1-21,1.94E-21,3.86E-22/
 DATA (PHI(J,3),J=1,07)/2*0.0,5*1.0/
 DATA (SIGMA(I,4),I=1,07)/1.62E-18,4.44E-19,1.19E-19,3.36E-20,8.79E
1-21,1.94E-21,3.86E-22/
 DATA (PHI(J,4),J=1,7)/3*1.0,4*0.0/
 DATA (SIGMA(I,5),I=1,8)/3.18E-20,3.25E-20,3.15E-20,2.34E-20,2.37E-
120,1.98E-20,8.37E-21,1.76E-21/
 DATA (PHI(J,5),J=1,8)/0.81,0.66,0.52,0.40,0.29,0.18,0.09,0.01/
 DATA (SIGMA(I,6),I=1,8)/3.18E-20,3.25E-20,3.15E-20,2.34E-20,2.37E-
120,1.98E-20,8.37E-21,1.76E-21/
 DATA (PHI(J,6),J=1,8)/0.19,0.34,0.48,0.60,0.71,0.82,0.91,0.99/
 DATA (SIGMA(I,7),I=1,09)/1.49E-20,9.94E-21,6.88E-21,4.97E-21,3.82E
1-21,3.01E-21,1.91E-21,1.15E-21,0.76E-21/
 DATA (PHI(J,7),J=1,9)/9*1.0/
 DATA (SIGMA(I,8),I=1,6)/4.66E-20,4.09E-20,2.96E-20,1.69E-20,6.92E-
121,1.34E-21/
 DATA (PHI(J,8),J=1,6)/0.987,0.722,0.663,0.474,0.300,0.123/
 DATA (SIGMA(I,09),I=1,31)/1.99E-22,3.60E-22,5.38E-22,7.48E-22,9.58
1E-22,1.31E-21,1.74E-21,2.20E-21,2.76E-21,3.31E-21,3.78E-21,4.54E-2
21,5.09E-21,4.93E-21,5.15E-21,5.52E-21,4.98E-21,4.17E-21,3.61E-21,3
3.18E-21,2.69E-21,2.17E-21,1.79E-21,1.52E-21,1.26E-21,9.77E-22,8.06
4E-22,6.76E-22,5.56E-22,4.84E-22,4.07E-22/
 DATA (PHI(J,09),J=1,31)/31*1.0/
 END
```

# Block Data MECH

```
 BLOCK DATA MECH
 COMMON /CALC/ NR,KR(77,5),A(77),S(77),R(77),ITYPE(77),IA(34),JA(21
18),DILUT,TEMP,ERR,START,STOPP,SPECIS(34),TPRNT,TSTEP
 DATA NR/76/
 DATA (KR(I,1),I=1,77)/1,3,4,1,1,5,1,6,6,2,7,7,8,8,9,9,10.4,4,11,11
1,8,4,12,13,13,13,13,13,14,12,12,24,24,2,2,2,2,2,27,28,20,18,27,28,
220,18,16,21,21,21,22,22,22,30,30,30,29,29,29,13,13,32,31,23,32,31,
323,26,19,25,17.15,32,31,23,0/
 DATA (KR(I,2),I=1,77)/0,0,2.4,3,2.5,0,0,1,7,0,1,2.2,9,0,0,0,0,0,4,
19,8,2,13,15,17,19,0,4,4,8,8,26,25,19,17,15,0,0,0.0,0,0,0.0,0,0,0,8
2,0,0,8,0,0,8,0,0,8,26,25.2,2,2.1,1,1,9,9,9,9,9,9,9,9,0/
 DATA (KR(I,3),I=1,77)/2,4,1,5.2,1,6,1,0,7,2,8,0,7,1.10,8,11,3,3,8,
19,8,13,14,14,14,14,14,21,8.8,25,26,1,1,1,1,1,21,22,21,21,29,9,30,2
22,21,0,9,9,0,15,23,0,17,31,0,19,32,14,14,19,17,15,12*0/
 DATA (KR(I,4),I=1,77)/3,4*0,1,0,5,0,7,1,2,0,0,8,0,8,0,0,0,8,0,0,0,
11,14,16,18,20,9,9,23,0,0,27,28,20,18,16,19,17,17,15,9,0,9,9,9,0,9,
20,0,9,0,0,9,0,0,9,0,27.28,1,1.1,12*0/
 DATA (KR(I,5),I=1,77)/29*0,22,22,21,45*0/
 DATA R/.35,4.4E+6,25.,.045,1.3E+4,1.3E+4,5600.,22...05,2.E-5,.001,
1.018,8000.,3000.,1200.,8400.,8.4E-4,9 5E-4,.019,8.7E+10,1.E+10,84.
2,2.4,2.5E+4,1000.,1.2E+4,1000.,1000.,1000.,1.E+5,.008,.008,1800.,1
3800.,1800.,1800.,1800.,1800.,1800.,7.5E+4,1.E+5,8000.,4000.,1.5E+5
4,3.E+5,1.E+5,8.E+4,8.E+4,.003,.001,1.5E+4,4.2E-6,9.8E-4,1.5E+4,6.E
5-5,.0025,4.5E+4,6.E-5,.0019,4.5E+4.1000.,1000.,800.,800.,800.,100.
6,100.,100.,4000.,4000.,4000.,4000.,4000.,4000.,4000.,4000.,0.0/
 DATA ITYPE/1,1.2,2,2,2,2,1,1,2,2.1,2,2,2,2,1,1,1,1.1,2,2,2,2,2,2,2
1,2,1,2,2,2,2,2,2,2,2,2,1,1,1,1,1,1,1,1,1,1,1,2,1,1,2,1,1,2,1,1,2,2
2,2,2,2,2,2,2,2.2,2,2,2,2,2,2,2,0/
 DATA IA/1,12,34,38,50,54,57,61,79,93,95,98,106,120,124,131,134,141
1,146,153,158,161,166,171,175,182,189,194,198,203,208,213,218,0/
 DATA JA/1.2,3,4,5,6,7,8,23,31,32,1,2,4,5,7,8.9,13,14,15,16,17,18,1
19,20,23,25,26,27,28,31,32,1,2,3,4,1,2,3,4,5,8,9,11,12,21,22,23,1,2
2,5,6,1,5,6,1,2,7,8,1,2,4,7,8,9,12,13,21,22,23,24,25,26,29,30,31,32
3,1,2,4,8,9,10,15,17,19,23,25,26,31,32,8,10,3,8,11,4,8,9,12,13,21,2
42,23,1,2,13,14,15,16,17,18,19,20,25,26,27,28,9,14,21,22,1,2,9,13,1
54,15,16,9,16,21,1,2,9,13,14,17,18,9,15,18,21,22,1,2,9,13,14,19,20,
69,17,20,21,30,8,9,21,8,9,15,22,23,1,2,9,15,23,8,24,25,26,1,2,9,13,
714,25,28,1,2,9,13,14,26,27,9,19,21,27,29,9,17,22,28,8,9,19,29,32,8
8,9,17,30,31,1,2,9,17,31,1,2,9,19,32,0/
 DATA SPECIS/4HNO2 ,4HNO  ,4HO   ,4HO3  ,4HNO3 ,4HN2O5,4HHONO,4HOH
1 ,4HHO2 ,4HHOOH,4HO1D ,4HPROP.4HADD ,4HX   ,4HMEO2,4HMEO ,4HC2O2,4
2HC2O ,4HC3O2,4HC3O ,4HHCHO,4HALD2,4HC2O3.4HBUT .4HSCO2,4HC4O2,4HC4
3O ,4HSCO ,4HALD4,4HALD3,4HC3O3.4HC4O3,4HM   ,4H    /
 END
```

# Block Data GEAR

```
      BLOCK DATA GEAR
      COMMON /GEAR5/ IW1(33,9)/GEAR7/IW2(660)
      DIMENSION IX1(200), IX2(200), IX3(200), IX4(60)
      EQUIVALENCE (IW2,IX1), (IW2(201),IX2), (IW2(401),IX3), (IW2(601),I
     1X4)
      DATA (IW1(I,1),I=1,33)/6,10,5,7,11,24,3,16,29,30,28,31,32,18,12,19
     1,26,4,23,20,25,27,8,1,2,9,13,14,15,17,21,22,0/
      DATA (IW1(I,2),I=1,33)/1,4,6,11,15,17,19,23,27,30,33,37,43,49,53,5
     16,63,69,76,84,88,94,98,112,130,147,170,179,187,194,202,211,218/
      DATA (IW1(I,3),I=1,33)/1,3,4,6,9,11,14,17,19,23,27,30,34,38,42,49,
     155,61,69,73,79,86,94,103,111,118,124,129,133,136,138,139,139/
      DATA (IW1(I,4),I=1,33)/1,3,4,6,9,11,14,17,19,23,27,30,34,38,42,49,
     155,61,69,73,79,86,94,95,96,97,98,99,100,101,102,102,0/
      DATA (IW1(I,5),I=1,33)/1,3,4,7,10,11,12,14,17,19,21,24,29,34,37,39
     1,45,49,53,58,64,68,72,78,85,91,97,102,106,109,111,112,112/
      DATA (IW1(I,6),I=1,33)/1,3,4,7,10,11,12,14,17,19,21,24,29,34,37,39
     1,45,49,53,58,64,68,72,78,85,91,97,102,106,109,111,111,0/
      DATA (IW1(I,7),I=1,33)/3,4,6,9,11,14,17,19,23,27,29,34,38,41,48,55
     1,61,68,73,79,85,94,102,110,117,123,128,132,135,137,138,139,0/
      DATA (IW1(I,9),I=1,33)/33,4*32,31,32,31,32,28,27,0,0,32,8*0,28,31,
     132,0,31,6*0/
      DATA IX1/1,3,24,2,26,1,3,18,24,25,4,23,24,25,5,18,6,23,5,7,18,24,8
     1,25,27,29,09,22,23,10,20,23,11,21,25,27,10,12,23,24,25,26,9,13,23,
     224,25,26,14,25,27,30,15,18,23,9,13,16,22,25,26,27,6,17,23,25,26,27
     3,7,15,18,23,24,25,26,15,18,19,23,24,25,26,32,16,20,25,27,6,21,23,2
     45,26,27,17,22,25,27,2,4,5,6,9,10,15,18,23,24,25,26,31,32,1,3,4,7,1
     52,13,16,17,18,19,21,23,24,25,26,27,29,30,3,4,7,12,13,16,17,18,19,2
     61,23,24,25,26,27,29,30,8,9,10,11,12,13,14,15,16,17,18,19,20,21,22,
     723,25,26,28,29,30,31,32,15,16,17,21,23,25,27,29,30,16,17,21,25,27,
     828,29,30,14,19,25,26,27,29,32,10,11,12,20,25,26,27/
      DATA IX2/30,8,14,15,18,20,22,23,28,31,11,14,15,18,23,28,32,3,24,23
     1,24,25,23,24,25,7,23,17,21,23,18,24,25,26,31,13,16,23,26,12,23,26,
     230,26,30,32,24,25,26,30,16,24,25,26,26,29,31,32,18,19,23,26,27,31,
     332,20,24,25,26,27,28,22,24,25,26,27,28,19,23,24,25,26,27,31,32,24,
     425,26,29,23,24,25,26,30,31,24,25,26,27,28,30,32,23,24,25,26,27,28,
     530,31,24,25,26,27,28,29,30,31,32,26,27,28,21,11,26,16,31,22,9,24,2
     65,18,4,23,26,15,27,31,32,19,6,21,17,9,10,12,13,24,25,7,18,3,1,4,23
     7,19,12,13,24,25,18,3,4,23,26,27,28,29,8,30,14,16,20,19,21,17,22,11
     8,12,13,24,25,18,23,26,2,29,30,16,19,21,17,12,13,24,25,27,28,29,8/
      DATA IX3/30,14,16,20,21,17,22,11,26,28,31,32,24,25,26,27,28,29,8,2
     14,25,26,27,28,30,14,23,26,31,23,26,29,32,19,231,210,109,225,3,24,2
     26,18,24,25,23,24,25,18,23,18,24,25,27,29,22,23,20,23,21,25,27,20,2
     33,24,25,26,22,23,24,25,26,25,27,30,18,23,22,23,24,25,26,27,23,25,2
     46,27,23,24,25,26,23,24,25,26,32,22,23,24,25,26,27,23,25,26,27,23,2
     55,26,27,24,25,26,27,31,32,25,26,27,29,30,31,32,26,27,29,30,31,32,2
     67,28,29,30,31,32,28,29,30,31,32,29,30,31,32,30,31,32,31,32,32,267,
     7188,205,228,255,102,73,256,189,254,223,232,230,76,172,237,191,276,
     8236,194,287,243,173,178,242,251,264,124,250,126,118,208,211,227,25
     93,229,190,259,129,260,258,82,280,294,195,286,265,84,186,104,197/
      DATA IX4/272,165,200,215,238,275,78,48,290,239,278,87,285,201,266,
     1284,77,135,72,288,300,291,95,137,92,246,158,249,292,159,162,161,30
     24,305,26*0/
      END
```

Function CIRC

```
      FUNCTION CIRC (TI,XI,YI)                                          AF   1
      DIMENSION XI(3), YI(3)                                            AF   2
      DX=XI(3)-XI(1)                                                    AF   3
      DY=YI(3)-YI(1)                                                    AF   4
      X=(XI(2)-XI(1))/DX                                                AF   5
      Y=(YI(2)-YI(1))/DY                                                AF   6
      T=(TI-XI(1))/DX                                                   AF   7
      IF (X.EQ.Y) GO TO 10                                              AF   8
      B=((X*X+Y*Y)*0.5-X)/(Y-X)                                         AF   9
      TT=SQRT(B*B+2.*T*(1.-B)-T*T)                                      AF  10
      CX=B+TT                                                           AF  11
      IF (X.GT.Y) CX=B-TT                                               AF  12
      IF (CX.LT.0..OR.CX.GT.1.) GO TO 10                                AF  13
    5 CIRC=CX*DY+YI(1)                                                  AF  14
      RETURN                                                            AF  15
   10 CX=T*Y/X                                                          AF  16
      IF (T.GT.X) CX=(T-X)*(1.-Y)/(1.-X)+Y                              AF  17
      GO TO 5                                                           AF  18
      END                                                               AF  19-
```

## Subroutine EMISS

```
      SUBROUTINE EMISS (NEM,EM,ESTRT,ESTOP,ESLP,EC)
      COMMON /GEAR6/ A(38,38),IX(38),SR(18)
      DIMENSION EM(11), EC(38), IFLAG(11)
      EM(NEM+1)=0.
      DO 5 I=1,11
      IFLAG(I)=3
      IF (I.LE.NEM.AND.ABS(EM(I)).EQ.0.) IFLAG(I)=0
      IF (I.LT.2.OR.I.GT.NEM-1) GO TO 5
      IF (EM(I-1).EQ.EM(I).AND.EM(I).EQ.EM(I+1)) IFLAG(I)=0
    5 CONTINUE
      IFLAG(1)=2
      IFLG1=1
      IF (EM(1).EQ.0..AND.EM(2).NE.0.) IFLG1=-1
      NEM1=NEM
      DO 10 I=1,NEM1
      IK=NEM1-I+1
      IF (EM(IK).GT.0.) GO TO 15
      NEM=NEM-1
   10 CONTINUE
   15 IF (NEM.EQ.0) RETURN
      IF (NEM.GT.1) GO TO 20
      ESLP=-EM(1)/1800.
      ESTOP=60.
      ESTRT=-60.*ESLP
      RETURN
   20 N=NEM
      NM1=NEM-1
      JK=4*N-2
      DO 25 I=1,JK
      EC(I)=0.
      DO 25 J=1,JK
   25 A(I,J)=0.0
C
C   LOOP THROUGH EACH HOUR TO SET UP A MATRIX
C
C   ... BUT FIRST SET UP FIRST HOUR (SPECIAL)
C
      A(1,1)=1.
      A(1,2)=60.
      DO 55 LM=1,3
      NM=NM1*(LM-1)+1
      DO 50 K=1,4
      IF (LM.EQ.1) A(NM,K+2)=-(60.**(K-1))
      IF (LM.EQ.2.AND.K.GT.1) A(NM,K+2)=-(FLOAT(K-1)*(60.**(K-2)))
      IF (LM.NE.3) GO TO 50
      IF (IFLG1.EQ.1) GO TO 45
      IF (EM(2)-EM(3)) 40,30,30
   30 DO 35 I=1,6
   35 A(NM-NM1,I)=0.
      A(NM-NM1,1)=1.
      GO TO 45
   40 A(NM,1)=1.
      GO TO 50
   45 IF (K.LE.2) GO TO 50
      A(NM,K+2)=-FLOAT(K-1)*(2.0**(K-3))*(60.**(K-3))
   50 CONTINUE
   55 CONTINUE
```

```
      IF (IFLG1.EQ.1.OR.EM(2).LT.EM(3)) A(N,2)=1.
      A(3*N-2,1)=60.
      A(3*N-2,2)=1800.
      EC(3*N-2)=EM(1)
C
C   NOW SET UP REST
C
      DO 125 I=2,NM1
      J=4*I-6
C
C   SET UP THIRD ORDER
C
      DO 65 LM=1,4
      M=LM-1
      NM=NM1*M+I
      T=FLOAT(I)*60.
      DO 60 K=1,4
      IF (LM.EQ.1) A(NM,J+K)=T**(K-1)
      IF (LM.EQ.2.AND.K.GT.1) A(NM,J+K)=FLOAT(K-1)*(T**(K-2))
      IF (LM.EQ.3.AND.K.GT.2) A(NM,J+K)=FLOAT(K-1)*(2.**(K-3))*(T**(K-3)
     1)
      IF (LM.EQ.4) A(NM,J+K)=(T**K-(T-60.)**K)/FLOAT(K)
      IF (LM.EQ.4) EC(NM)=EM(I)
      IF (LM.NE.4) A(NM,J+K+4)=-A(NM,J+K)
   60 CONTINUE
   65 CONTINUE
C
C   NOW RESET A MATRIX ACCORDING TO THE
C          RESPECTIVE ORDER
C
      IF (IFLAG(I).EQ.3) GO TO 125
      KL=4-IFLAG(I)
      DO 120 L=2,KL
      K=4*I-L
      IK=I+NM1*(4-L)
      IF (L.EQ.4) GO TO 75
      DO 70 II=1,JK
      IF (L.EQ.2) A(IK-1,II)=0.
      IF (L.NE.2) A(IK,II)=0.
   70 A(II,K)=0.
      IF (L.EQ.2) A(IK-1,K)=1.
      IF (L.NE.2) A(IK,K)=1.
      GO TO 120
   75 CONTINUE
      IF (IFLAG(I-1)-1) 80,90,100
   80 DO 85 II=1,JK
      IF (I.NE.2) A(IK-1,II)=0.
      IF (I.EQ.2) A(IK+NM1-1,II)=0.
   85 A(II,K)=0.
      IF (I.EQ.2) A(IK+NM1-1,K)=1.
      IF (I.NE.2) A(IK-1,K)=1.
      GO TO 120
   90 DO 95 II=1,JK
      A(II,K)=0.
   95 A(IK+NM1-2,II)=0.
      A(IK+NM1-2,K)=1.
      GO TO 120
```

```
  100 DO 110 II=1,JK
      IF (I.NE.2) GO TO 105
      IF (IFLG1.EQ.1) GO TO 105
      IF (EM(2).LT.EM(3)) A(IK+NM1-1,II)=0.
      IF (EM(2).GE.EM(3)) A(NM1*2+1,II)=0.
      A(II,K)=0.
      GO TO 110
  105 A(II,K)=0.
      A(IK+NM1-1,II)=0.
  110 CONTINUE
      IF (I.NE.2) GO TO 115
      IF (IFLG1.EQ.1) GO TO 115
      IF (EM(2).LT.EM(3)) A(IK+NM1-1,K)=1.
      IF (EM(2).GE.EM(3)) A(NM1*2+1,K)=1.
      GO TO 120
  115 A(IK+NM1-1,K)=1.
  120 CONTINUE
  125 CONTINUE
C
C  SET LAST EMISSION VALUE EQUAL TO ZERO
C
      T=FLOAT(N)*60.
      DO 130 I=1,4
      L=JK-4+I
      A(JK-1,L)=(T**I-(T-60.)**I)/FLOAT(I)
  130 A(JK,L)=T**(I-1)
      EC(JK-1)=EM(N)
C
      CALL DEC (JK,38,A,IX,IER)
      CALL SOL (JK,38,A,EC,IX)
C
      IF (IFLG1.EQ.-1.OR.EM(2).EQ.0.) GO TO 135
      IF (EC(1).LT.0.) IFLG1=-1
      IF (IFLG1.EQ.-1) GO TO 20
  135 DO 170 I=2,NM1
      ISAV=IFLAG(I)
      IR=ISAV+1
      T1=FLOAT(I-1)*60.+1.
      T2=FLOAT(I)*60.-1.
      IF (I.LE.3.AND.EM(1).GE.0.) IFLG1=1
      J=4*I-2
      GO TO (165,140,145 150),IR
  140 VAL1=EC(J-3)+EC(J-[illegible]*T1
      VAL2=EC(J-3)+EC(J-2)*T2
      EMI=AMIN1(VAL1,VAL2)
      GO TO 160
  145 TI=-EC(J-2)/(2.0*EC(J-1))
      EMI=999.
      IF (TI.LT.T1.OR.TI.GT.T2) GO TO 155
      EMI=(EC(J-1)*TI+EC(J-2))*TI+EC(J-3)
      GO TO 155
  150 IF (EC(J).EQ.0.) GO TO 170
      EMI=999.
      DETR=(EC(J-1)**2)-3.*EC(J)*EC(J-2)
      IF (DETR.LT.0.) GO TO 155
      DETR=SQRT(DETR)
      Z1=(-EC(J-1)+DETR)/(3.0*EC(J))
      Z2=-(EC(J-1)+DETR)/(3.0*EC(J))
      Z=-1.
      IF (Z2.GT.FLOAT(I-1)*60..AND.Z2.LT.FLOAT(I)*60.) Z=Z2
      IF (Z1.GT.FLOAT(I-1)*60..AND.Z1.LT.FLOAT(I)*60.) Z=Z1
      IF (Z.LT.0.) GO TO 155
      EMI=((Z*EC(J)+EC(J-1))*Z+EC(J-2))*Z+EC(J-3)
  155 VAL1=((T1*EC(J)+EC(J-1))*T1+EC(J-2))*T1+EC(J-3)
      VAL2=((T2*EC(J)+EC(J-1))*T2+EC(J-2))*T2+EC(J-3)
      EMI=AMIN1(VAL1,VAL2,EMI)
  160 IF (EMI.LT.0.) IFLAG(I)=IFLAG(I)-1
  165 IF (IFLAG(I).NE.ISAV) GO TO 20
  170 CONTINUE
C
      ESTRT=EC(1)
      ESLP=EC(2)
      ESTOP=FLOAT(N)*60.
      RETURN
      END
```

# Subroutine CONVT

```
      SUBROUTINE CONVT (NUM,L)
C
C     SUBROUTINE CONVT CONVERTS INTEGERS TO ALPHANUMERIC FOR
C   PRINTING
C
C   ASSUMES VALUE OF INTEGER IS POSITIVE
C
      DIMENSION L(3), JDIGIT(10)
C
      DATA JDIGIT/1H0,1H1,1H2,1H3,1H4,1H5,1H6,1H7,1H8,1H9/
      DATA JBLANK/1H /
C
      N=NUM
      DO 5 I=1,3
      L(I)=JBLANK
    5 CONTINUE
C
      DO 10 K=1,3
      I=4-K
      NEXT=N/10
      NDX=(N-NEXT*10)+1
      L(I)=JDIGIT(NDX)
      NK=K
      IF (NEXT.LE.0) GO TO 15
      N=NEXT
   10 CONTINUE
C
C
   15 RETURN
      END
```

## Subroutine EDGMX

```
      SUBROUTINE EDGMX (X,Y,N,XMX,YMX,L)
      DIMENSION X(N), Y(N)
      LL=N-1
      IF (N.LE.2) GO TO 10
      NGO=0
      DO 5  I=2,LL
      IF(Y(I).GT.Y(I-1)) GO TO 5
      IF(Y(I).GT.Y(I+1)) L=I+1
      IF(Y(I).GT.Y(I+1)) NGO=1
    5 CONTINUE
      IF(NGO.EQ.1) GO TO 13
   10 XMX=X(N)
      YMX=Y(N)
      L=N-1
      RETURN
   13 L=MAX0(L-1,3)
      X21=X(L-1)-X(L-2)
      X221=X(L-1)*X(L-1)-X(L-2)*X(L-2)
      X32=X(L)-X(L-1)
      XL2=X(L)*X(L)
      Y21=Y(L-1)-Y(L-2)
      C=(Y21/X21-(Y(L)-Y(L-1))/X32)/(X221/X21-(XL2-X(L-1)*X(L-1))/X32)
      B=(Y21-C*X221)/X21
      A=Y(L)-B*X(L)-C*XL2
      XMX=-B*0.5/C
      YMX=A+B*XMX+C*XMX*XMX
      IF (XMX.GE.0.999*X(L)) YMX=Y(L)
      IF (YMX.EQ.Y(L)) XMX=X(L)
      IF (XMX.LT.1.001*X(L-2).AND.L.GT.3) GO TO 13
      L=L-1
      IF (XMX.LE.X(L)) L=L-1
      RETURN
      END
```

# Subroutine DEC

```
      SUBROUTINE DEC (N,ND,A,IP,IER)
      DIMENSION A(ND,N), IP(N)
      L=N
      IER=0
      IP(L)=1
      IF (L.EQ.1) GO TO 30
      NM1=L-1
      DO 25 K=1,NM1
      K1=K+1
      M=K
      DO 5 I=K1,L
    5 IF (ABS(A(I,K)).GT.ABS(A(M,K))) M=I
      IP(K)=M
      T=A(M,K)
      IF (M.EQ.K) GO TO 10
      IP(L)=-IP(L)
      A(M,K)=A(K,K)
      A(K,K)=T
   10 IF (T.EQ.0.) GO TO 35
      T=1./T
      DO 15 I=K1,L
   15 A(I,K)=-A(I,K)*T
      DO 25 J=K1,L
      T=A(M,J)
      A(M,J)=A(K,J)
      A(K,J)=T
      IF (T.EQ.0.) GO TO 25
      DO 20 I=K1,L
      A(I,J)=A(I,J)+A(I,K)*T
   20 CONTINUE
   25 CONTINUE
   30 K=L
      IF (A(L,L).EQ.0.) GO TO 35
      RETURN
   35 IER=K
      IP(L)=0
      RETURN
      END
```

## Subroutine SOL

```
      SUBROUTINE SOL (L,ND,A,B,J)
      DIMENSION A(ND,L), B(L), J(L)
      N=L
      IF (N.EQ.1) GO TO 15
      DO 5 K=2,N
      M=J(K-1)
      C=B(M)
      B(M)=B(K-1)
      B(K-1)=C
      DO 5 I=K,N
      B(I)=B(I)+A(I,K-1)*C
    5 CONTINUE
      K=N
      DO 10 KB=2,N
      B(K)=B(K)/A(K,K)
      C=B(K)
      K=K-1
      DO 10 I=1,K
      B(I)=B(I)-A(I,K+1)*C
   10 CONTINUE
   15 B(1)=B(1)/A(1,1)
      RETURN
      END
```

# Subroutine VVLBLF

```
      SUBROUTINE VVLBLF (X2,Y2)
C
C     *** SETS A LINE LABEL INTO A VECTOR PLOT PROVIDING THAT
C         A CALL TO SUBROUTINE PLTLBL HAS PRESET THE NECESSARY
C         PARAMETERS IN /VVLBL/
C              GW LUNDBERG/SAI  DEC ;77
C
C     X2,Y2      THE TERMINAL POINT OF THE CURRENT VECTOR
C                IN INCHES FROM PRESENT PLOT ORIGIN
C
C     *** NOTES --
C         (1) THERE ARE THREE ENTRY POINTS -- VVLBLF SETS UP THE
C             PARAMETERS FOR VVLBLC WHICH ACTUALLY DOES THE LABELING.
C             VVLBLL CLEANS UP IN CASE THERE WAS NOT ENOUGH
C             ROOM FOR THE LAST LABEL
C         (2) THE LABELS ARE SEPERATED BY DIST INCHES EXCEPT FOR
C             THE FIRST LABEL WHICH STARTS FACT*DIST INCHES FROM
C             THE BEGINNING OF THE VECTOR PLOT -- THIS PROVIDES FOR
C             STAGGERED LABELS.
C
      DIMENSION XSV(20), YSV(20)
C
C     *** DIST IS THE DISTANCE IN INCHES BETWEEN LABELS.  FACT
C         IS THE FACTOR (0-1) OF DIST TO USE FOR THE FIRST LABEL.
C         CHRSZ IS THE SIZE OF THE LABEL CHARACTERS IN INCHES.
C         NCHR IS THE NUMBER OF CHARACTERS (0-10), AND LABEL
C         IS THE A-FORMATED TEXT OF THE LABEL
      COMMON /VVLBL/ FACT,DIST,CHRSZ,NCHR,OZL
      DATA MXSV/20/
C
C     *** MOVE THE PEN TO THE FIRST POINT
      CALL PLOT (X2,Y2,3)
C
C     *** IF THERE ARE TO BE NO LABELS -- JUST RETURN
      IF (NCHR.EQ.0) RETURN
C
C     *** SET UP THE OFFSET NECESSARY TO CENTER THE LABEL AND
C         THE DISTANCE REQUIRED BY THE LABEL
      OFF=CHRSZ/2.
      SZLBL=NCHR*CHRSZ+2.*OFF-0.3*CHRSZ
C
C     *** INITALIZE THE ACCUMULATED LENGTH OF THE VECTORS, THE
C         LENGTH REQUIRED BEFORE FIRST LABEL, AND THE NUMBER
C         OF SAVED POINTS (VECTORS) THAT MAY HAVE BEEN PREEMPTED
C         BY THE LABEL
      TOTSZ=0.
      SKPSZ=FACT*DIST
      NSV=0
C
C     *** REMEMBER THE STARTING LOCATION OF FIRST VECTOR
      X1=X2
      Y1=Y2
C
      RETURN
C
C*************************************************************
C                       ENTRY VVLBLC
```

```
C**********************************************************************
C
      ENTRY VVLBLC(X2,Y2)
C
C     *** IF THERE ARE TO BE NO LABELS -- PLOT THE VECTOR AND RETURN
      IF (NCHR.GT.0) GO TO 5
      CALL PLOT (X2,Y2,2)
      RETURN
C
C     *** IF SEEKING ROOM FOR THE LABEL -- SKIP FOLLOWING
    5 IF (NSV.GT.0) GO TO 15
C
C     *** CALCULATE THIS VECTOR LENGTH AND ADD TO THE ACCUMULATED
C         LENGTH.  IF A LABEL IS TO START IN THIS VECTOR, SKIP TO
C         120, ELSE PLOT THE VECTOR AND RETURN
      VECSZ=SQRT((X2-X1)**2+(Y2-Y1)**2)
      TOTSZ=TOTSZ+VECSZ
      IF (TOTSZ.GT.SKPSZ) GO TO 10
      CALL PLOT (X2,Y2,2)
      X1=X2
      Y1=Y2
      RETURN
C
C     *** ITS TIME FOR A LABEL -- LOCATE START
   10 RATIO=(VECSZ-TOTSZ+SKPSZ)/VECSZ
      X1L=X1+RATIO*(X2-X1)
      Y1L=Y1+RATIO*(Y2-Y1)
C
C     *** PLOT SUBVECTOR AND REMEMBER THE END POINT
      CALL PLOT (X1L,Y1L,2)
      X1=X1L
      Y1=Y1L
C
C     *** FIND OUT IF THERE IS ENOUGH ROOM LEFT IN THIS VECTOR
C         FOR THE LABEL -- IF THERE ISNT, SAVE (X2,Y2) AND RETURN
   15 HAVSZ=SQRT((X2-X1L)**2+(Y2-Y1L)**2)
      IF (HAVSZ.GE.SZLBL) GO TO 20
      NSV=NSV+1
C
C     *** CHECK FOR OVERFLOW
      IF (NSV.GT.MXSV) STOP
      XSV(NSV)=X2
      YSV(NSV)=Y2
      X1=X2
      Y1=Y2
      RETURN
C
C     *** CALCULATE THE END OF THE LABEL
C         IM SURE THERE IS AN EASIER WAY TO DO THIS, BUT IT
C         ESCAPES ME
   20 A=(X2-X1)**2+(Y2-Y1)**2
      B=-2*((X1L-X1)*(X2-X1)+(Y1L-Y1)*(Y2-Y1))
      C=(X1L-X1)**2+(Y1L-Y1)**2-SZLBL*SZLBL
C
      SQRTD=SQRT(B*B-4*A*C)
      T1=(-B+SQRTD)/(2*A)
      T2=(-B-SQRTD)/(2*A)
```

```
C
C     *** PICK THE MINIMUM T BETWEEN 0-1 (MUST BE ONE)
      IF (T1.LT.0.) T1=1.
      IF (T2.LT.0.) T2=1.
      RATIO=AMIN1(T1,T2)
C
C     *** SET LABEL END POINT
      X2L=X1+RATIO*(X2-X1)
      Y2L=Y1+RATIO*(Y2-Y1)
C
C     *** CALCULATE LABEL ANGLE
      DX=X2L-X1L
      DY=Y2L-Y1L
      ANG=0.
      IF (DY.NE.0.) ANG=ATAN2(DY,DX)
C
      XL=X1L
      YL=Y1L
      COSA=COS(ANG)
      SINA=SIN(ANG)
C
C     *** REVERSE EVERYTHING IF ANGLE IN QUADRANTS 2 OR 3
      IF (DX.GE.0.) GO TO 25
      XL=X2L
      YL=Y2L
      COSA=-COSA
      SINA=-SINA
      IF (DY.GE.0.) ANG=ANG-3.1415926536
      IF (DY.LT.0.) ANG=ANG+3.1415926536
   25 ANGD=ANG*180./3.1415926536
C
C     *** LOCATE AND PLOT LABEL
      XL=XL+OFF*COSA+OFF*SINA
      YL=YL+OFF*SINA-OFF*COSA
      IDG=NCHR-2
      CALL NUMBER (XL,YL,CHRSZ,OZL,ANGD,IDG)
C
C     *** FINISH OFF THIS SEGMENT BY MEANS OF A PSUEDO REENTRY
      TOTSZ=0.
      SKPSZ=DIST
      NSV=0
      X1=X2L
      Y1=Y2L
      CALL PLOT (X1,Y1,3)
      GO TO 5
C
C***************************************************************
C                 ENTRY VVLBLL
C***************************************************************
C
      ENTRY VVLBLL(X2,Y2)
C
C     *** PLOT THE SAVED VECTORS IF ANY
      IF (NSV.EQ.0) RETURN
      DO 30 I=1,NSV
      CALL PLOT (XSV(I),YSV(I),2)
      CONTINUE
      NSV=0
      RETURN
C
      END
```

## Subroutine NEWLIN

```
      SUBROUTINE NEWLIN (N,OT,HCT,SX,NS,NE,NL,NR,XNL,NPL,TOL,NUL,NTL,II)
      COMMON /NEED/ HC,XN,NN,NB,R(20),OZP(20),OZN(8,20),RHO(8,20),M,OC(4
     1),OS(2),HCS,XNS,LL,HCLL(8)
      DIMENSION XNL(20), OT(20), HCT(20), YP(20), TM(20), NUL(20), NTL(2
     10)
      IT=1
      ISAV=0
      IF (OT(N-1).LT.TOL*OT(N)) GO TO 5
      IF (N.LE.2) GO TO 5
      DO 1 I=NS,NE
      J=NE-I+NS
      IF(OZP(J).LE.OT(N).AND.OZP(J).GE.OT(N-1)) GO TO 5
    1 CONTINUE
      N=N-1
    5 CALL CURV1 (N,OT,HCT,SP1,SP2,YP,TM,SX)
      DO 15 I=NS,NE
      IF (OZP(I).GT.OT(N)) GO TO 20
      IF (OZP(I).LT.OT(1).AND.NL.GE.6) GO TO 20
      IF (NL.LT.6) GO TO 10
      IF (IT.GT.0) NUL(I)=NUL(I)+1
      IF(IT.LT.0.AND.ISAV.NE.1) NUL(ISAV)=NUL(ISAV)-1
      IF (NUL(I).EQ.1) NTL(I)=II
      IF (NUL(I).EQ.1) NUL(I)=II
   10 XNL(I-NR)=CURV2(OZP(I),N,OT,HCT,YP,SX,IT)
      IF (IT.GT.0) GO TO 15
      ISAV=I
      SX=SX*10.
      SX=AMAX1(-50.,SX)
      GO TO 5
   15 IT=2
      I=NE+1
   20 NPL=I-1
      RETURN
      END
```

# APPENDIX C

# SELECTED FLOW DIAGRAMS

This appendix contains flow diagrams for some of the important routines of the OZIPP program. The diagrams are listed as follows:

| Routine in OZIPP | | Page Number |
|---|---|---|
| Program | MAIN | 192 |
| Subroutine | RLINE | 194 |
| Subroutine | PHOT | 197 |
| Subroutine | SIM | 198 |
| Subroutine | DIFFUN | 199 |
| Subroutine | OZMX | 200 |
| Subroutine | LINER | 201 |

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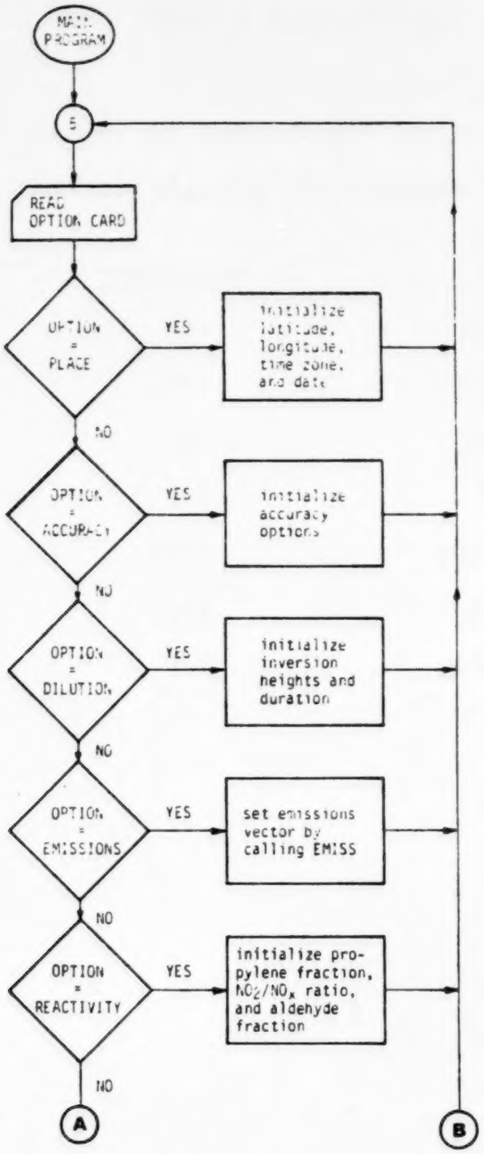
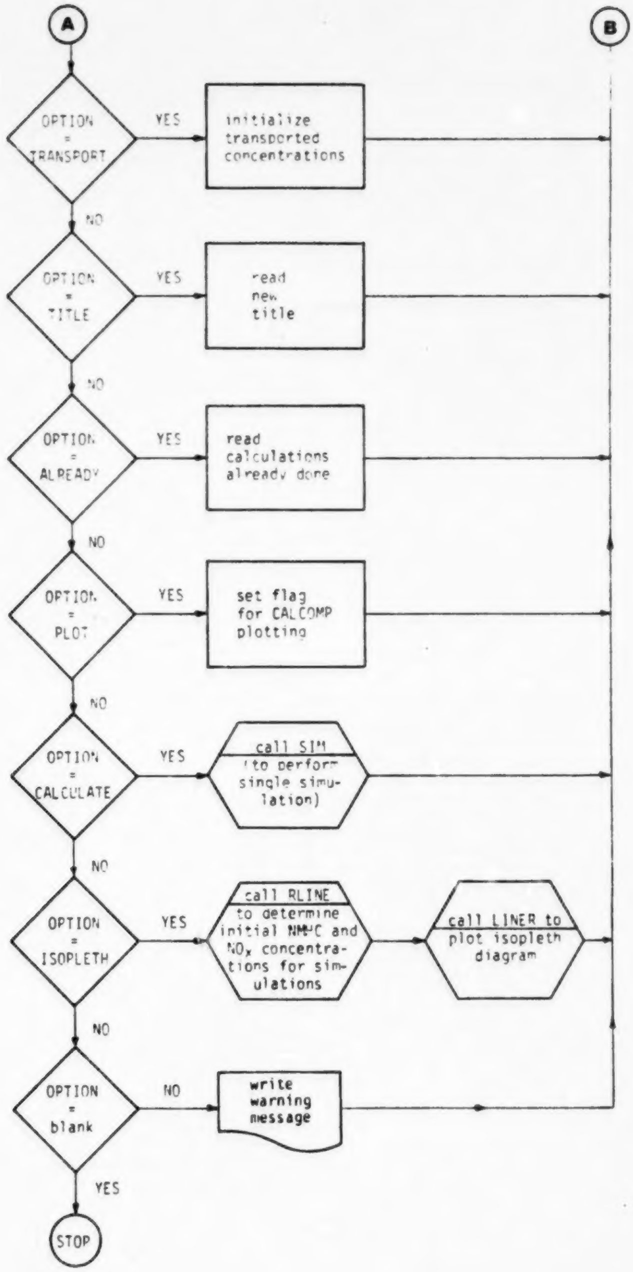
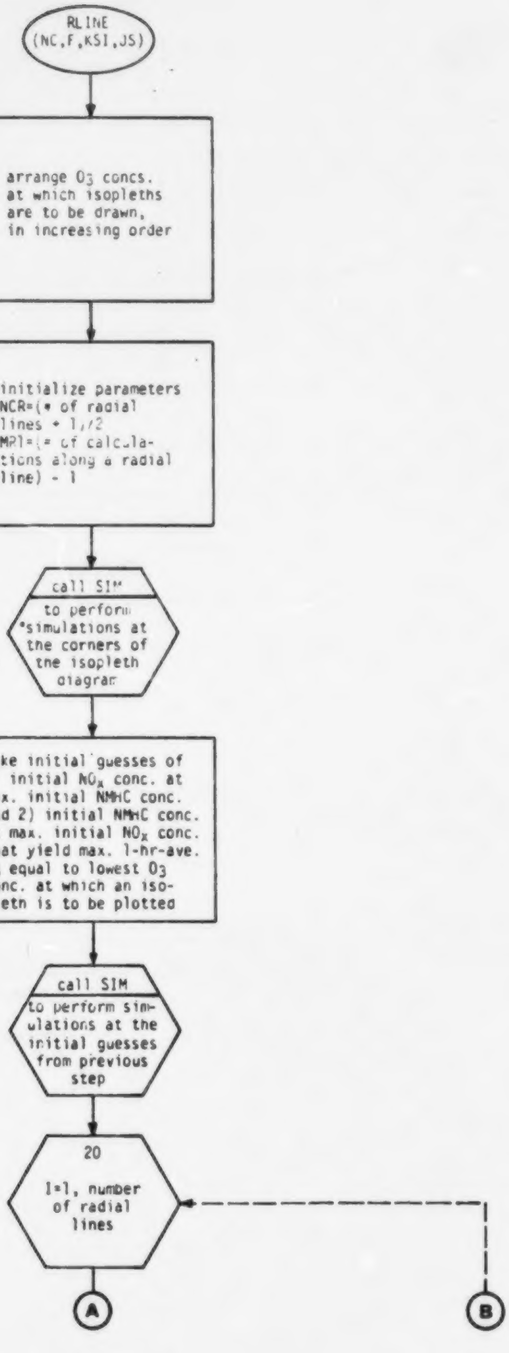

MAIN PROGRAM
5
READ OPTION CARD
OPTION = PLACE
YES
initialize latitude, longitude, time zone, and date
NO
OPTION = ACCURACY
YES
initialize accuracy options
NO
OPTION = DILUTION
YES
initialize inversion heights and duration
NO
OPTION = EMISSIONS
YES
set emissions vector by calling EMISS
NO
OPTION = REACTIVITY
YES
initialize propylene fraction, NO2/NOx ratio, and aldehyde fraction
NO
A
B

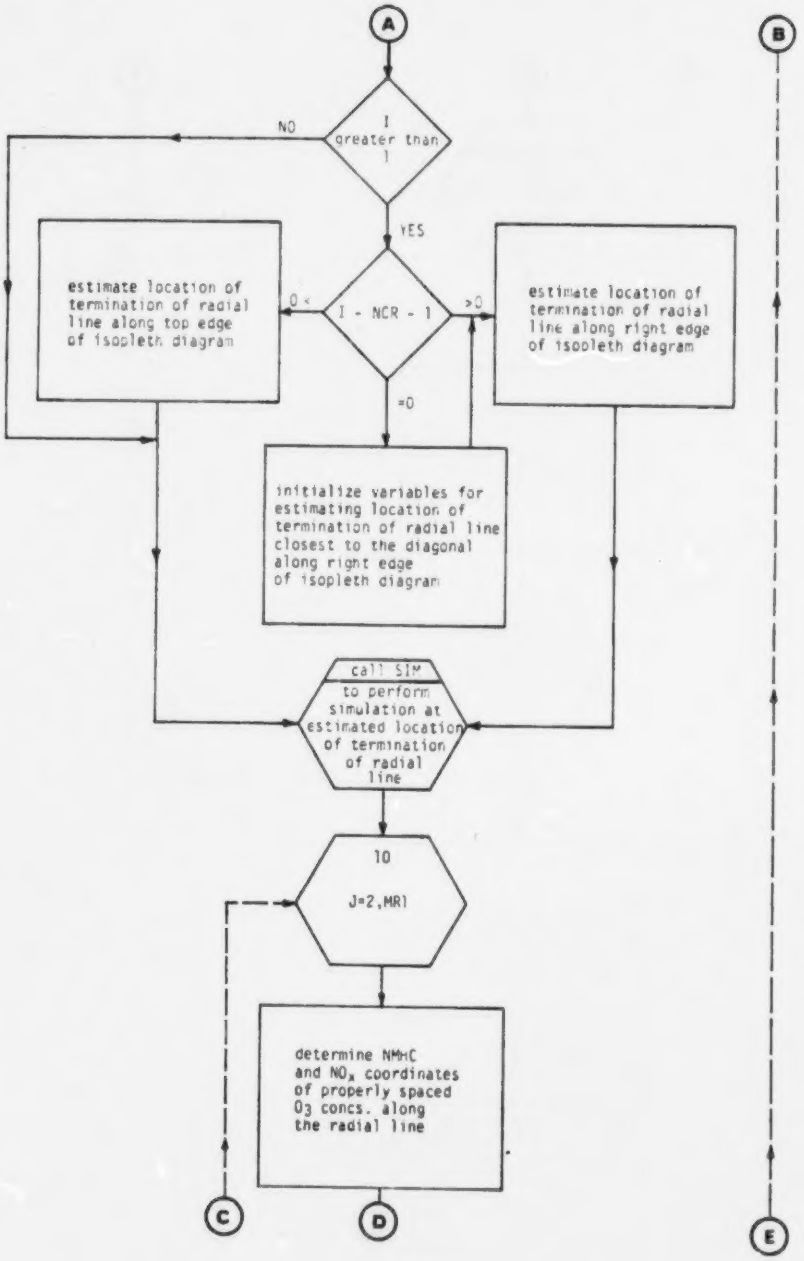
Flow diagram of the MAIN program, which processes the options, reads input data, and calls subroutines as required.


A
B
OPTION = TRANSPORT
YES
initialize transported concentrations
NO
OPTION = TITLE
YES
read new title
NO
OPTION = ALREADY
YES
read calculations already done
NO
OPTION = PLOT
YES
set flag for CALCOMP plotting
NO
OPTION = CALCULATE
YES
call SIM (to perform single simulation)
NO
OPTION = ISOPLETH
YES
call RLINE to determine initial NMHC and NOx concentrations for simulations
call LINER to plot isopleth diagram
NO
OPTION = blank
NO
write warning message
YES
STOP

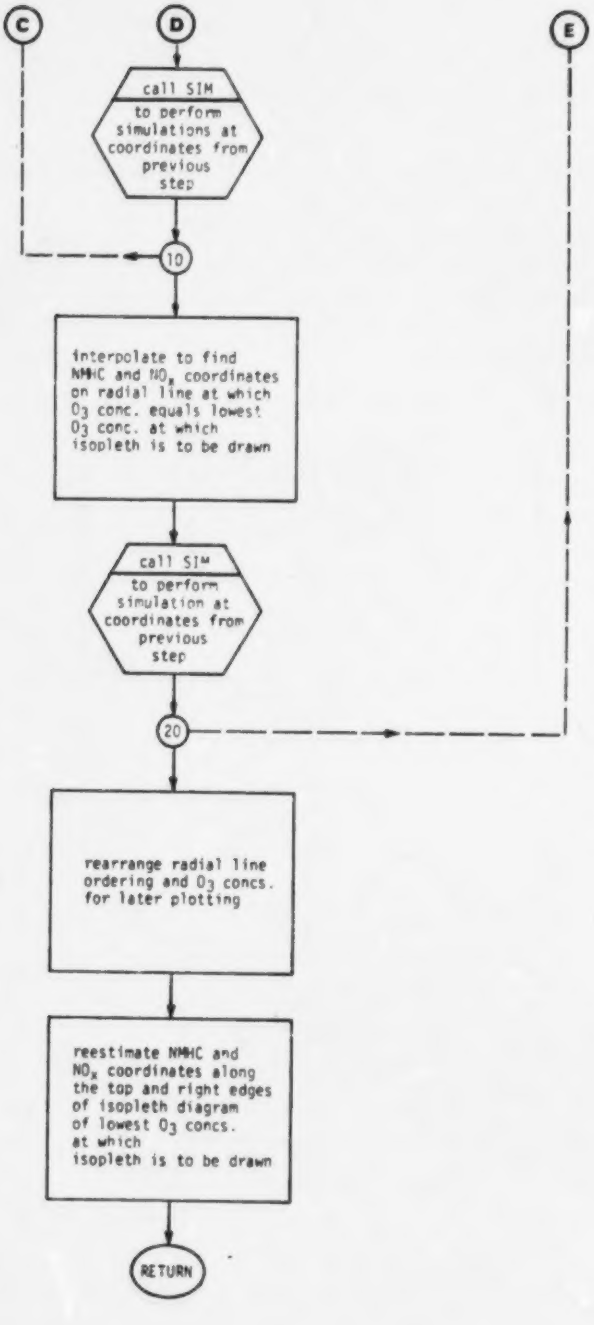
MAIN (Concluded)


RLINE
(NC,F,KSI,JS)
arrange $O_3$ concs. at which isopleths are to be drawn, in increasing order
initialize parameters NCR=(# of radial lines + 1)/2 MP1=(# of calculations along a radial line) - 1
call SIM
to perform simulations at the corners of the isopleth diagram
make initial guesses of 1) initial $NO_x$ conc. at max. initial NMHC conc. and 2) initial NMHC conc. at max. initial $NO_x$ conc. that yield max. 1-hr-ave. $O_3$ equal to lowest $O_3$ conc. at which an isopleth is to be plotted
call SIM
to perform simulations at the initial guesses from previous step
20
I=1, number of radial lines
A
B

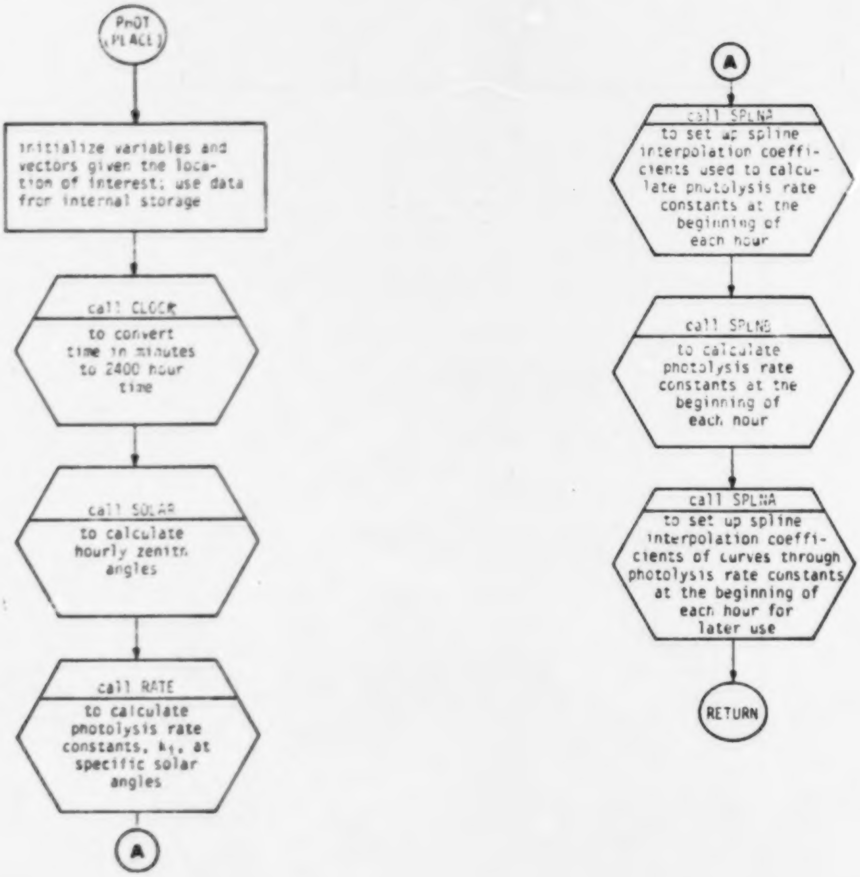
Flow diagram of subroutine RLINE, which performs the calculations for the location of the ozone value on the isopleth diagram


A
B
I greater than 1
NO
YES
estimate location of termination of radial line along top edge of isopleth diagram
0 <
I - NCR - 1
>0
estimate location of termination of radial line along right edge of isopleth diagram
=0
initialize variables for estimating location of termination of radial line closest to the diagonal along right edge of isopleth diagram
call SIM
to perform simulation at estimated location of termination of radial line
10
J=2,MR1
determine NMHC and NO$_x$ coordinates of properly spaced O$_3$ concs. along the radial line
C
D
E

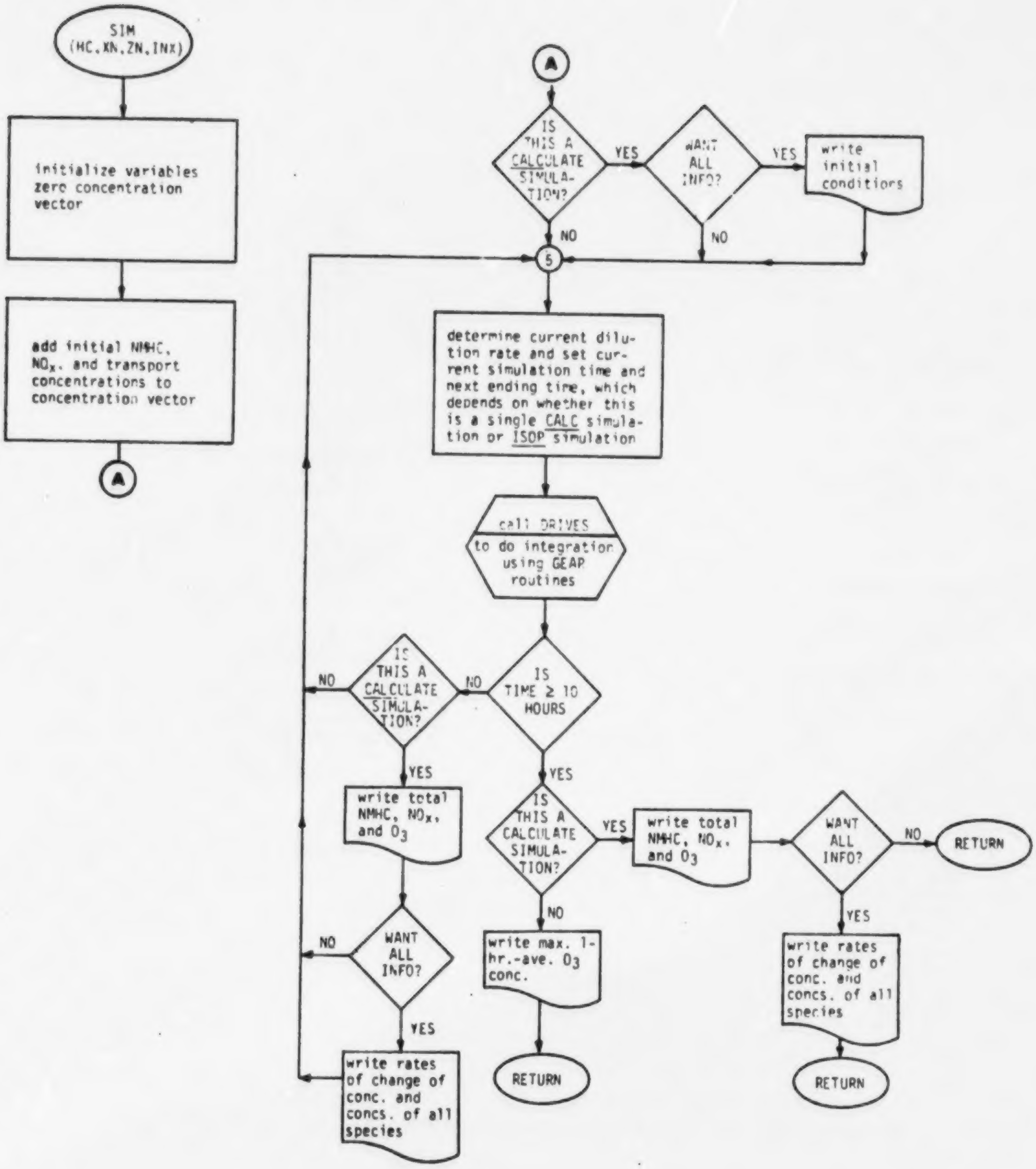
RLINE (Continued)


C
D
E
call SIM
to perform simulations at coordinates from previous step
10
interpolate to find NMHC and $NO_x$ coordinates on radial line at which $O_3$ conc. equals lowest $O_3$ conc. at which isopleth is to be drawn
call SIM
to perform simulation at coordinates from previous step
20
rearrange radial line ordering and $O_3$ concs. for later plotting
reestimate NMHC and $NO_x$ coordinates along the top and right edges of isopleth diagram of lowest $O_3$ concs. at which isopleth is to be drawn
RETURN

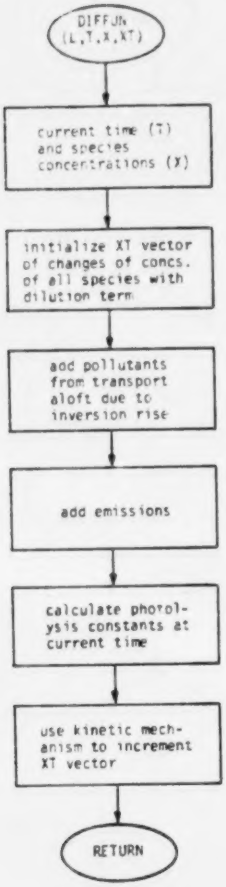
RLINE (Concluded)


PHOT
(PLACE)
initialize variables and vectors given the location of interest; use data from internal storage
call CLOCK
to convert time in minutes to 2400 hour time
call SOLAR
to calculate hourly zenith angles
call RATE
to calculate photolysis rate constants, $k_i$, at specific solar angles
A
A
call SPLNA
to set up spline interpolation coefficients used to calculate photolysis rate constants at the beginning of each hour
call SPLNB
to calculate photolysis rate constants at the beginning of each hour
call SPLNA
to set up spline interpolation coefficients of curves through photolysis rate constants at the beginning of each hour for later use
RETURN

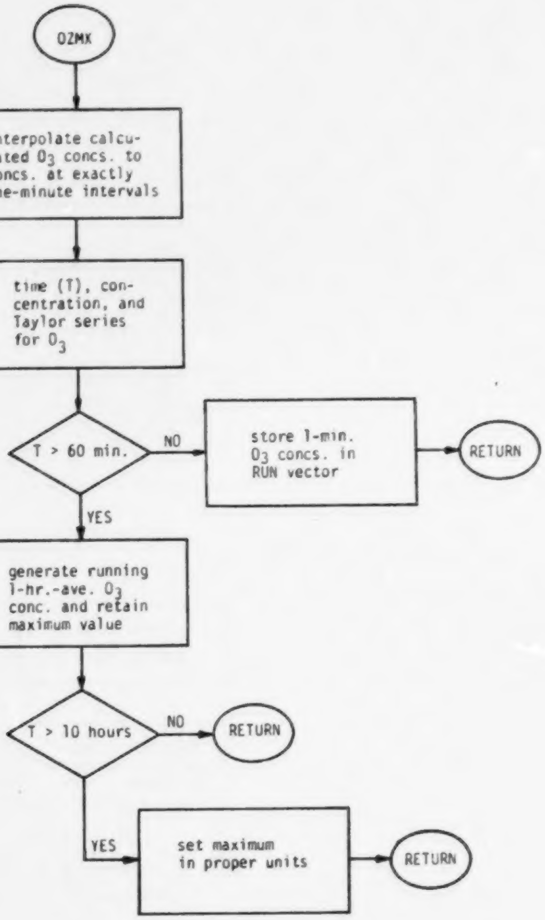
Flow diagram of subroutine PHOT, which directs calculations of photolysis rate constants


SIM (HC,XN,ZN,INX)
initialize variables zero concentration vector
add initial NMHC, NO$_x$, and transport concentrations to concentration vector
A
A
IS THIS A CALCULATE SIMULATION?
YES
WANT ALL INFO?
YES
write initial conditions
NO
NO
5
determine current dilution rate and set current simulation time and next ending time, which depends on whether this is a single CALC simulation or ISOP simulation
call DRIVES to do integration using GEAP routines
IS TIME ≥ 10 HOURS
NO
IS THIS A CALCULATE SIMULATION?
NO
YES
write total NMHC, NO$_x$, and O$_3$
WANT ALL INFO?
NO
YES
write rates of change of conc. and concs. of all species
YES
IS THIS A CALCULATE SIMULATION?
YES
write total NMHC, NO$_x$, and O$_3$
WANT ALL INFO?
NO
RETURN
YES
write rates of change of conc. and concs. of all species
RETURN
NO
write max. 1-hr.-ave. O$_3$ conc.
RETURN

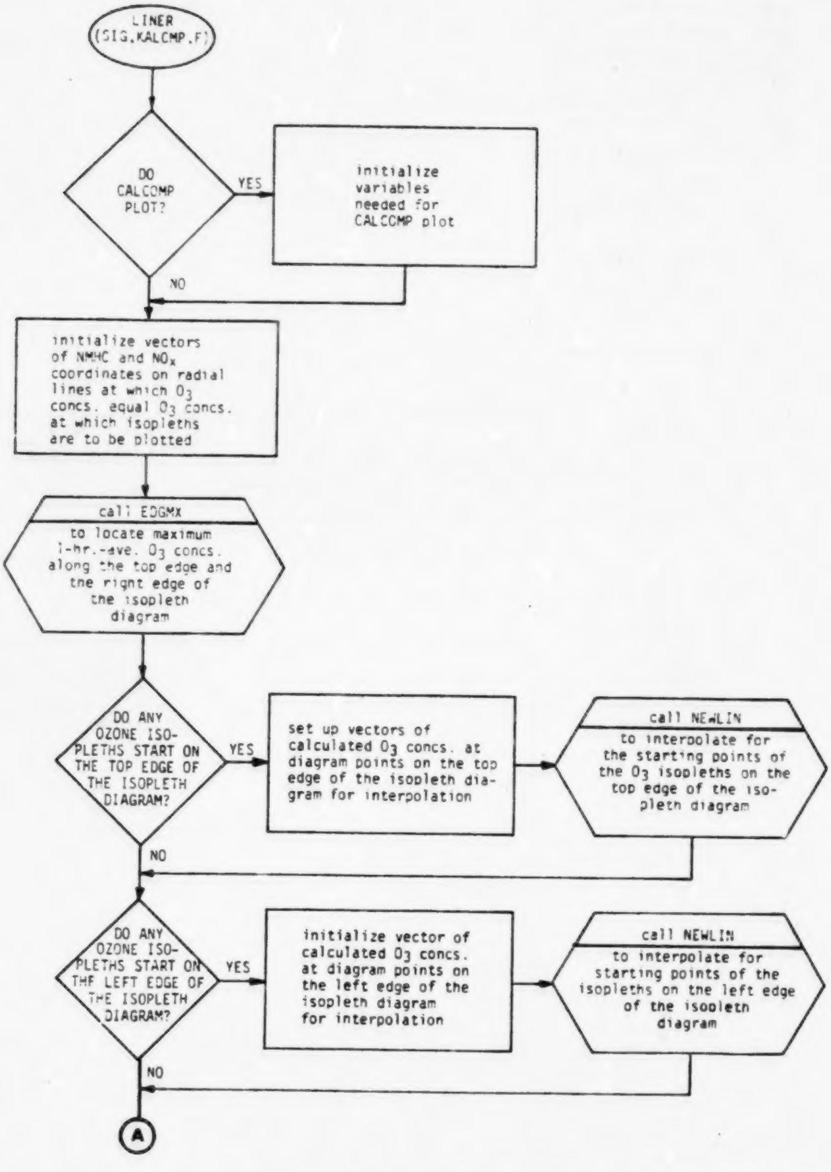
Flow diagram of subroutine SIM, which controls each calculation of the maximum one-hour average ozone concentration


DIFFUN
(L,T,X,XT)
current time (T) and species concentrations (X)
initialize XT vector of changes of concs. of all species with dilution term
add pollutants from transport aloft due to inversion rise
add emissions
calculate photolysis constants at current time
use kinetic mechanism to increment XT vector
RETURN

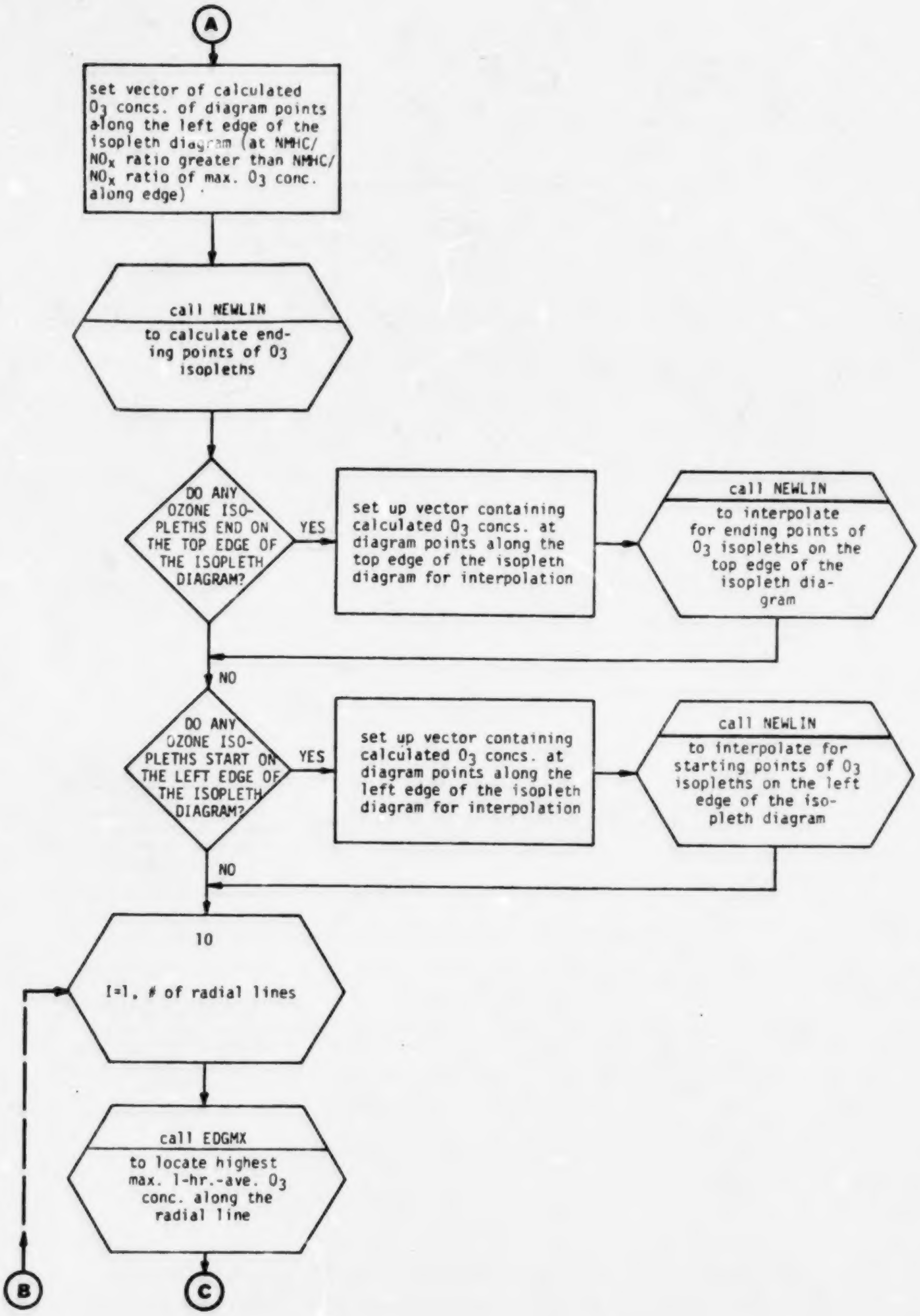
Flow diagram of subroutine DIFFUN, which updates the concentration vector based on current dilution rate (if any), emissions (if any), and chemical reactions in the kinetic mechanism. The XT vector is the vector of rates of change for each species.


OZMX
interpolate calculated O3 concs. to concs. at exactly one-minute intervals
time (T), concentration, and Taylor series for O3
T > 60 min.
NO
store 1-min. O3 concs. in RUN vector
RETURN
YES
generate running 1-hr.-ave. O3 conc. and retain maximum value
T > 10 hours
NO
RETURN
YES
set maximum in proper units
RETURN

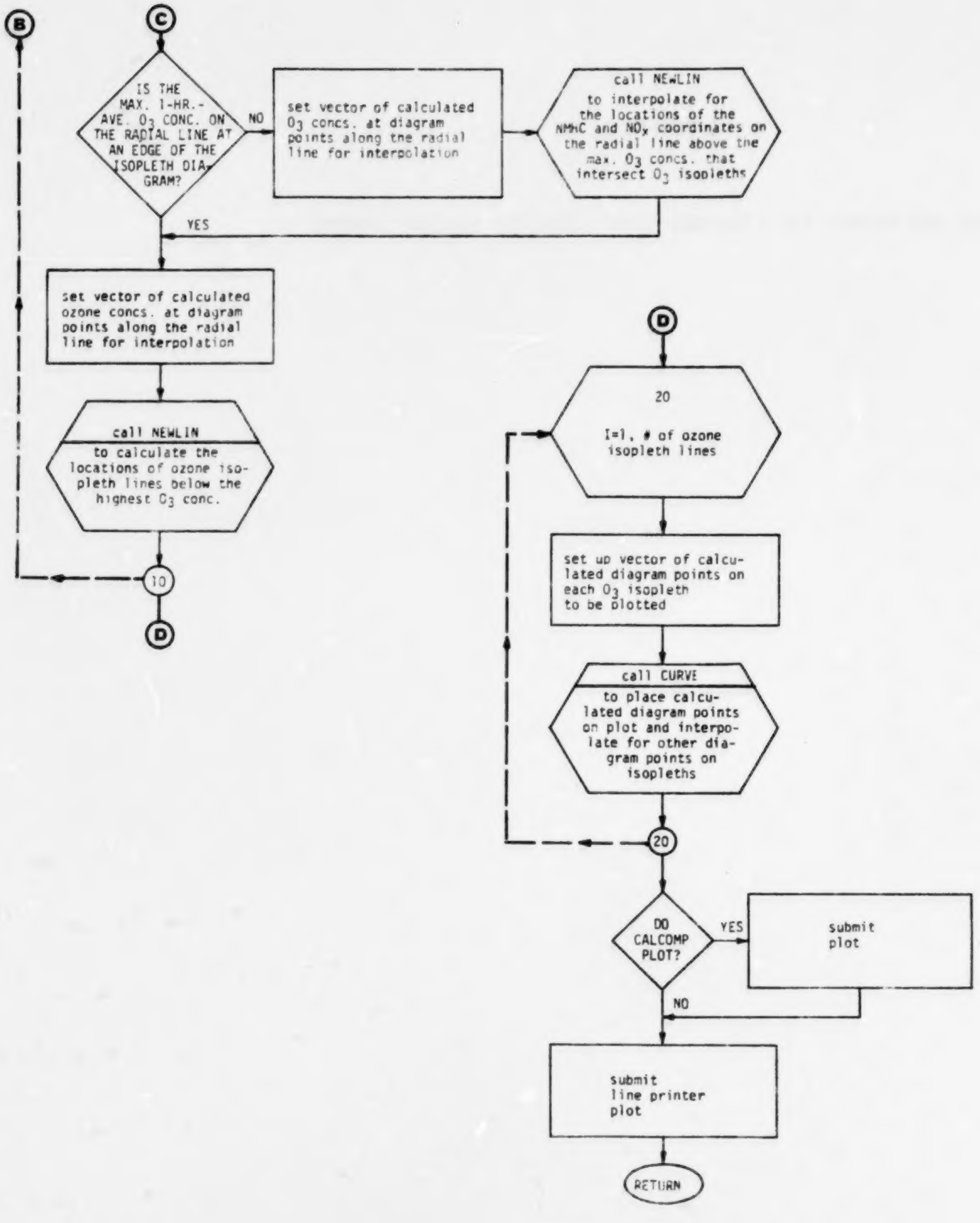
Flow diagram of subroutine OZMX, which monitors interpolation for maximum one-hour average ozone concentration


LINER (SIG,KALCMP,F)
DO CALCOMP PLOT?
YES
initialize variables needed for CALCOMP plot
NO
initialize vectors of NMHC and $NO_x$ coordinates on radial lines at which $O_3$ concs. equal $O_3$ concs. at which isopleths are to be plotted
call EDGMX
to locate maximum 1-hr.-ave. $O_3$ concs. along the top edge and the right edge of the isopleth diagram
DO ANY OZONE ISOPLETHS START ON THE TOP EDGE OF THE ISOPLETH DIAGRAM?
YES
set up vectors of calculated $O_3$ concs. at diagram points on the top edge of the isopleth diagram for interpolation
call NEWLIN
to interpolate for the starting points of the $O_3$ isopleths on the top edge of the isopleth diagram
NO
DO ANY OZONE ISOPLETHS START ON THE LEFT EDGE OF THE ISOPLETH DIAGRAM?
YES
initialize vector of calculated $O_3$ concs. at diagram points on the left edge of the isopleth diagram for interpolation
call NEWLIN
to interpolate for starting points of the isopleths on the left edge of the isopleth diagram
NO
A

Flow diagram of subroutine LINER, which calculates the desired ozone isopleths and submits the isopleth diagram to the line printer


A
set vector of calculated O3 concs. of diagram points along the left edge of the isopleth diagram (at NMHC/NOx ratio greater than NMHC/NOx ratio of max. O3 conc. along edge)
call NEWLIN
to calculate ending points of O3 isopleths
DO ANY OZONE ISOPLETHS END ON THE TOP EDGE OF THE ISOPLETH DIAGRAM?
YES
set up vector containing calculated O3 concs. at diagram points along the top edge of the isopleth diagram for interpolation
call NEWLIN
to interpolate for ending points of O3 isopleths on the top edge of the isopleth diagram
NO
DO ANY OZONE ISOPLETHS START ON THE LEFT EDGE OF THE ISOPLETH DIAGRAM?
YES
set up vector containing calculated O3 concs. at diagram points along the left edge of the isopleth diagram for interpolation
call NEWLIN
to interpolate for starting points of O3 isopleths on the left edge of the isopleth diagram
NO
10
I=1, # of radial lines
call EDGMX
to locate highest max. 1-hr.-ave. O3 conc. along the radial line
B
C

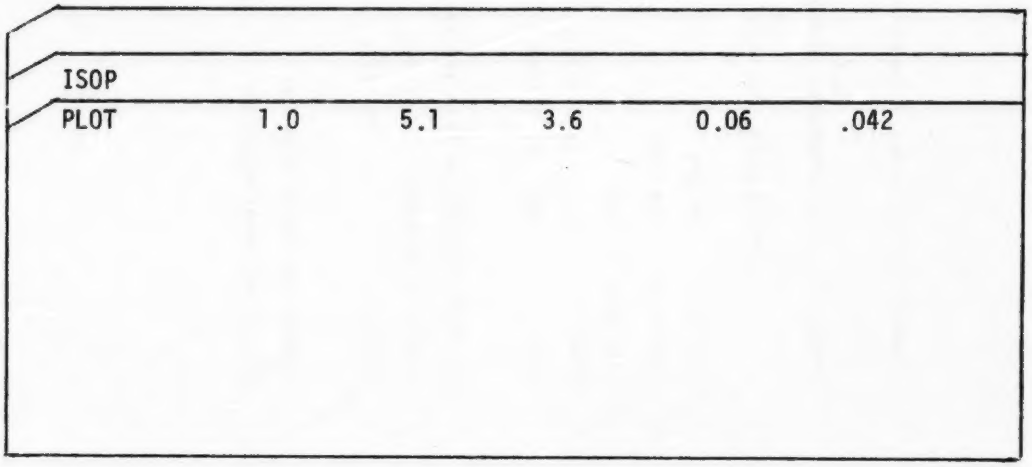
LINER (Continued)


B
C
IS THE MAX. 1-HR.-AVE. $O_3$ CONC. ON THE RADIAL LINE AT AN EDGE OF THE ISOPLETH DIAGRAM?
NO
set vector of calculated $O_3$ concs. at diagram points along the radial line for interpolation
call NEWLIN
to interpolate for the locations of the NMHC and $NO_x$ coordinates on the radial line above the max. $O_3$ concs. that intersect $O_3$ isopleths
YES
set vector of calculated ozone concs. at diagram points along the radial line for interpolation
call NEWLIN
to calculate the locations of ozone isopleth lines below the highest $O_3$ conc.
10
D
D
20
I=1, # of ozone isopleth lines
set up vector of calculated diagram points on each $O_3$ isopleth to be plotted
call CURVE
to place calculated diagram points on plot and interpolate for other diagram points on isopleths
20
DO CALCOMP PLOT?
YES
submit plot
NO
submit line printer plot
RETURN

LINER (Concluded)

# APPENDIX D

## INPUT AND OUTPUT FOR STANDARD OZONE ISOPLETH DIAGRAM EXAMPLE



```
ISOP
PLOT             1.0        5.1        3.6         0.06       .042
```

FIGURE D-1.  Input Deck For Standard Diagram Example.

```
STANDARD OZONE ISOPLETH CONDITIONS

PHOTOLYTIC RATE CONSTANTS CALCULATED FOR

        LOS ANGELES, CALIF.

LATITUDE     34.058
LONGITUDE    118.250
TIME ZONE    8.0
DATE         6     21    1975
TIME         800   TO    1800     LOCAL DAYLIGHT TIME

DILUTION DETERMINED FROM THE FOLLOWING
INVERSION HEIGHTS     INITIAL   510.     FINAL       630.
TIMING                START     800.     STOP       1500.

INITIAL PROPYLENE FRACTION     .250      NO2/NOX    .250
INITIAL ALDEHYDE FRACTION      .050
```

FIGURE D-2. Output For Standard Diagram Example

```
THE FOLLOWING SIMULATIONS WERE DONE.

     HC               NOX              RATIO            OZONE
   .00000           .00000            .00000           .00000
   .00000           .28000            .00000           .00555
  2.00000           .28000           7.14286           .44847
  2.00000           .00000            .00000           .00000
   .66667           .28000           2.38095           .11901 NOT MAX
  2.00000           .04995          40.04220           .20551
  1.29978           .18197           7.14286           .34608 NOT MAX
   .64989           .09098           7.14286           .22120 NOT MAX
   .32494           .04549           7.14286           .13778 NOT MAX
   .16312           .02284           7.14286           .08438 NOT MAX
  1.70176           .28000           6.07771           .42742 NOT MAX
  1.11933           .18417           6.07771           .32946 NOT MAX
   .55966           .09208           6.07771           .20832 NOT MAX
   .27983           .04604           6.07771           .12884 NOT MAX
   .15290           .02516           6.07771           .08348 NOT MAX
  1.40352           .28000           5.01256           .38897 NOT MAX
   .94517           .18856           5.01256           .30236 NOT MAX
   .48953           .09766           5.01256           .19473 NOT MAX
   .25368           .05061           5.01256           .12349 NOT MAX
   .14632           .02919           5.01256           .08329 NOT MAX
  1.10528           .28000           3.94742           .31779 NOT MAX
   .78290           .19833           3.94742           .25539 NOT MAX
   .44563           .11289           3.94742           .17657 NOT MAX
   .24930           .06315           3.94742           .11971 NOT MAX
   .14941           .03785           3.94742           .08416 NOT MAX
```

FIGURE D-2 (Continued)

```
  .80704      .28000      2.88227      .19098 NOT MAX
  .64926      .22526      2.88227      .16956 NOT MAX
  .43902      .15232      2.88227      .13525 NOT MAX
  .29267      .10154      2.88227      .10644 NOT MAX
  .20113      .06978      2.88227      .08514 NOT MAX
  .65791      .28000      2.34970      .11512 NOT MAX
  .60070      .25565      2.34970      .11080 NOT MAX
  .49420      .21033      2.34970      .10168 NOT MAX
  .39923      .16991      2.34970      .09204 NOT MAX
  .32049      .13639      2.34970      .08274 NOT MAX
 2.00000      .22789      8.77622      .41815
 1.32272      .15072      8.77622      .32424
  .66136      .07536      8.77622      .20904 NOT MAX
  .33068      .03768      8.77622      .13121 NOT MAX
  .17574      .02002      8.77622      .08409 NOT MAX
 2.00000      .17578     11.37803      .38096
 1.35389      .11899     11.37803      .30000
  .68604      .06029     11.37803      .19389
  .34511      .03033     11.37803      .12355 NOT MAX
  .19605      .01723     11.37803      .08367 NOT MAX
 2.00000      .12367     16.17260      .32704
 1.40654      .08697     16.17260      .26557
  .75213      .04651     16.17260      .17910
  .40261      .02489     16.17260      .11912
  .24082      .01489     16.17260      .08508 NOT MAX
 2.00000      .07155     27.95069      .24923
 1.50541      .05386     27.95069      .21295
  .89159      .03190     27.95069      .15645
  .52248      .01869     27.95069      .11138
```

FIGURE D-2 (Continued)

```
   .34191        .01223        27.95069        .08526 NOT MAX
  2.00000        .03681        54.32763        .17397
  1.69696        .03032        54.32763        .15810
  1.12259        .02066        54.32763        .12835
   .76637        .01411        54.32763        .10284
   .54949        .01011        54.32763        .08362
   .54090        .28000         1.93177        .06282
  2.00000        .01354       147.71556        .09819
```

FIGURE D-2 (Continued)

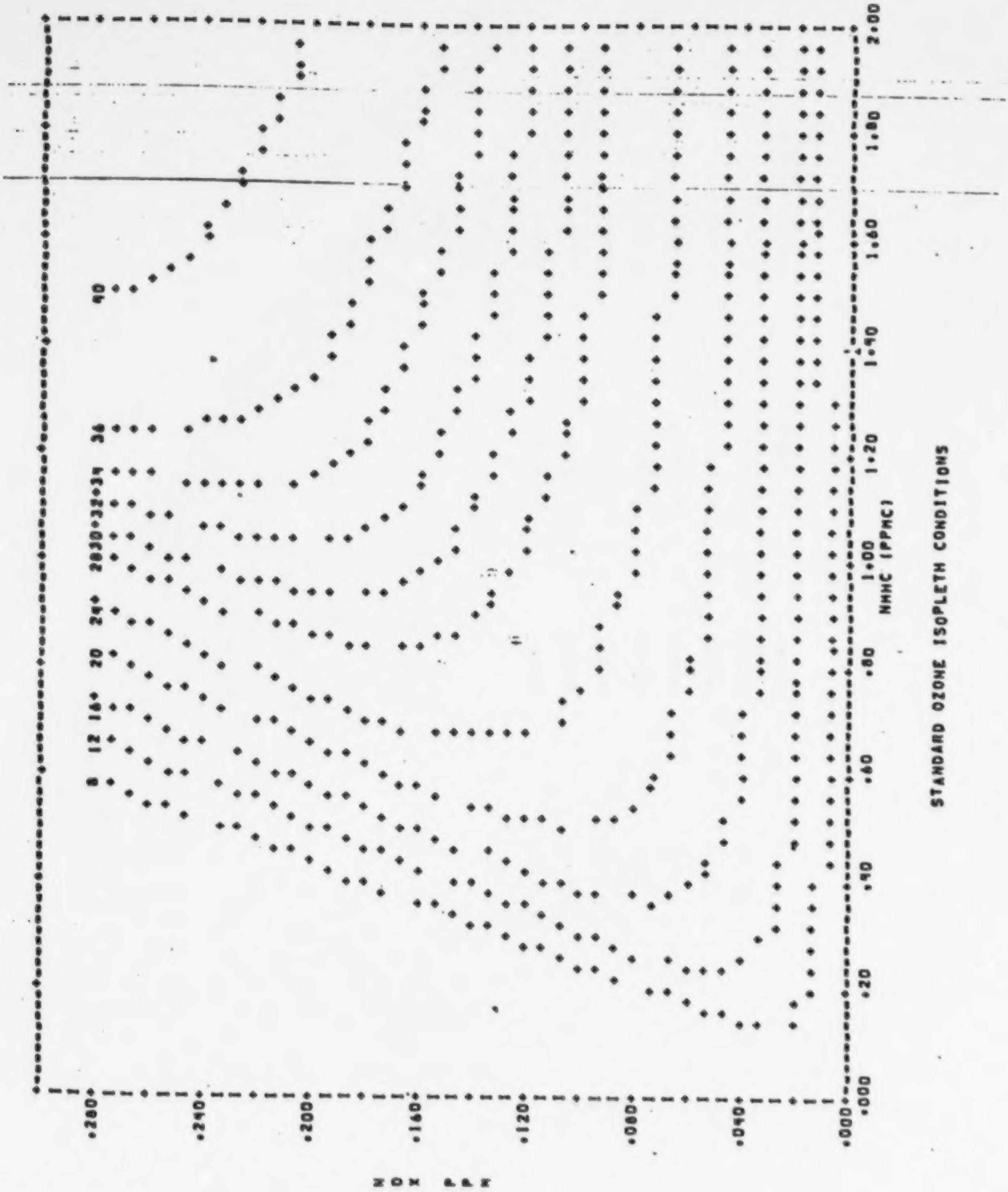


FIGURE D-2 (Continued)

```
THE OZONE LINES ARE    .08000  .12000  .16000  .20000  .24000  .28000  .30000  .32000  .34000  .36000
                       .40000
```

FIGURE D-2 (Continued)

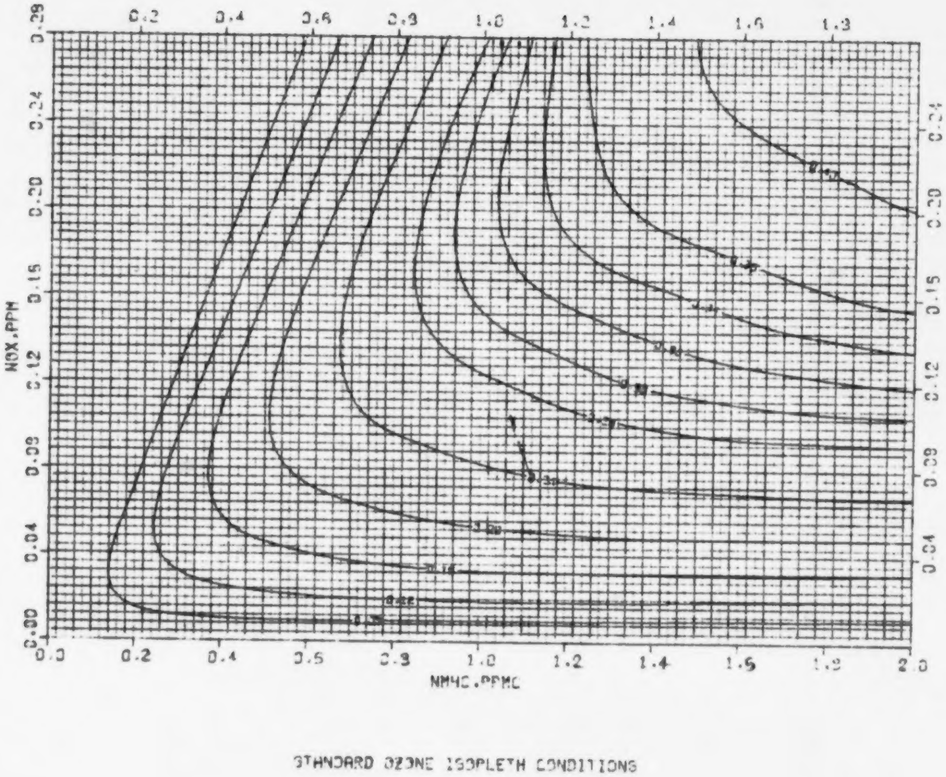
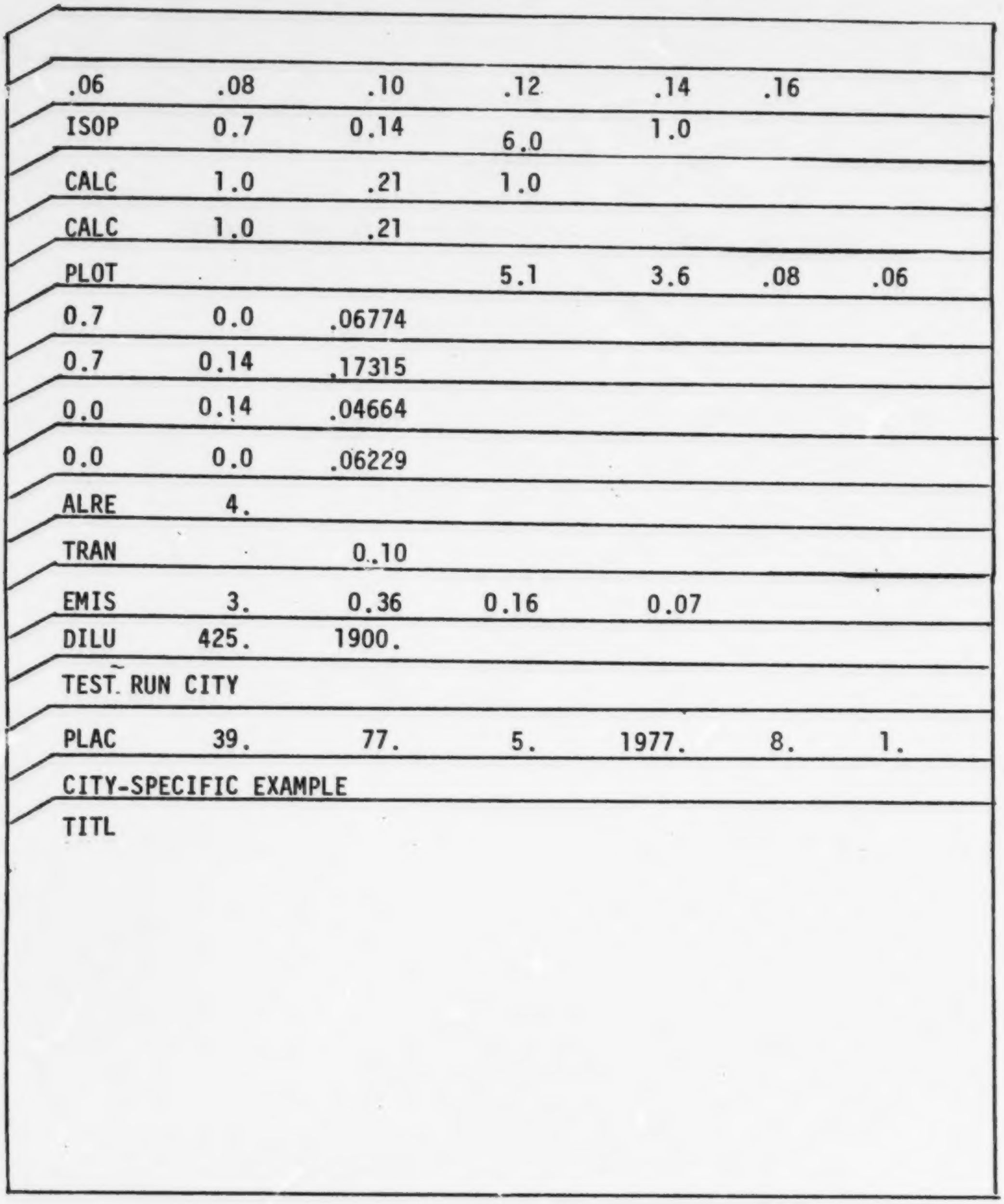


FIGURE D-3. CALCOMP Plot For Standard Diagram Example.

# APPENDIX E

# INPUT AND OUTPUT FOR CITY-SPECIFIC DIAGRAM EXAMPLE



```
.06      .08      .10      .12      .14      .16
ISOP     0.7      0.14     6.0      1.0
CALC     1.0      .21      1.0
CALC     1.0      .21
PLOT                       5.1      3.6      .08      .06
0.7      0.0      .06774
0.7      0.14     .17315
0.0      0.14     .04664
0.0      0.0      .06229
ALRE     4.
TRAN              0.10
EMIS     3.       0.36     0.16     0.07
DILU     425.     1900.
TEST RUN CITY
PLAC     39.      77.      5.       1977.    8.       1.
CITY-SPECIFIC EXAMPLE
TITL
```

FIGURE E-1. Input Deck For City-specific Diagram Example.

```
THE FOLLOWING RESULTS WERE READ IN.

      HC              NOX             RATIO            OZONE
    .00000          .00000           .00000           .06729
    .00000          .14000           .00000           .04664
    .70000          .14000          5.00000           .17315
    .70000          .00000           .00000           .06774
```

Figure E-2 Output For City-Specific Diagram Example

```
CITY-SPECIFIC EXAMPLE


PHOTOLYTIC RATE CONSTANTS CALCULATED FOR


        TEST RUN CITY


LATITUDE      39.000

LONGITUDE      77.000

TIME ZONE     5.0

DATE          8      1    1977

TIME          800   TO    1800     LOCAL DAYLIGHT TIME

SOLAR NOON    1314


DILUTION DETERMINED FROM THE FOLLOWING

INVERSION HEIGHTS       INITIAL    425.      FINAL      1900.

TIMING                  START      800.      STOP       1500.


INITIAL PROPYLENE FRACTION     .250      NO2/NOX    .250

INITIAL ALDEHYDE FRACTION      .050


TRANSPORTED CONCENTRATIONS

ALOFT                   OZONE      .100      HYDROCARBON   .000     NOX    .000 PPM


CONTINUOUS EMISSIONS (EXPRESSED AS THE FRACTION OF

INITIAL NON-BACKGROUND CONCENTRATION EMITTED PER HOUR)

HOUR         1      2      3

FRACTION   .360   .160   .070
```

Figure E-2 (continued)

```
                         CITY-SPECIFIC EXAMPLE

  TIME       HC       PROPYLENE     ALDEHYDE      NOX          NO2        OZONE
 (LDT )     TOTAL     FRACTION      FRACTION     TOTAL      FRACTION    (INSTANT)

  800.     1.00000      .25000       .05000      .21000      .25000      .00000

  900.     1.06317      .23397       .07178      .22767      .39099      .00831

 1000.      .88886      .20057       .11404      .19618      .65288      .03020

 1100.      .67768      .15350       .16177      .15052      .83232      .08668

 1200.      .48401      .10062       .19604      .10230      .88829      .14797

 1300.      .34851      .05925       .20207      .06590      .90567      .18170

 1400.      .25300      .03202       .18766      .04052      .91155      .19317

 1500.      .18558      .01693       .16519      .02425      .91387      .19051

 1600.      .16996      .00877       .14308      .01772      .92390      .20001

 1700.      .15888      .00490       .12599      .01338      .93572      .20517

 1800.      .15209      .00314       .11533      .01080      .95242      .20742

  MAXIMUM OZONE NOT REACHED, THE LAST ONE HOUR AVERAGE WAS .20645 PPM.
```

Figure E-2 (continued)

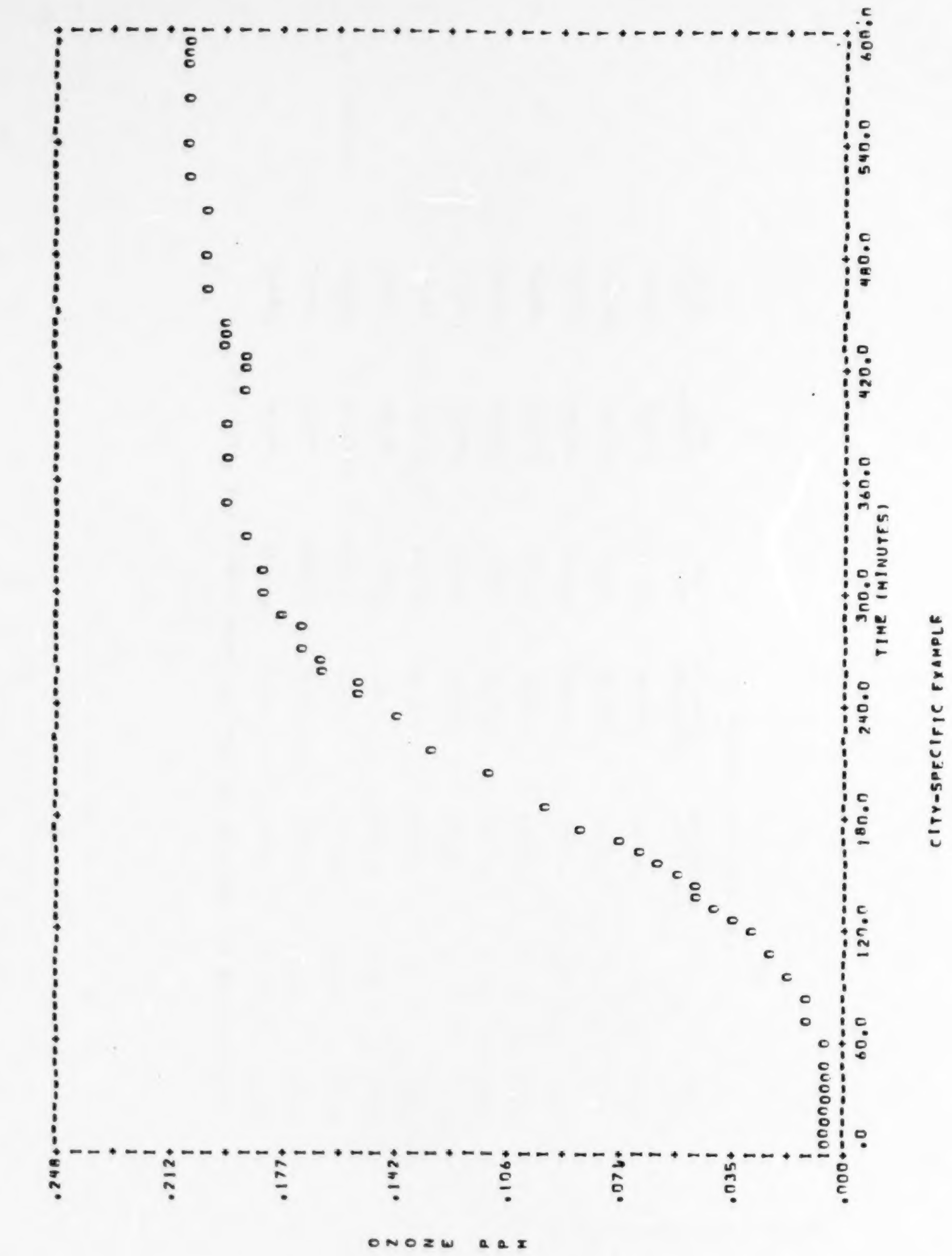


Figure E-2 (continued)

```
CITY-SPECIFIC EXAMPLE

PHOTOLYTIC RATF CONSTANTS CALCULATED FOR

        TEST RUN CITY

LATITUDE      39.000
LONGITUDE      77.000
TIME ZONE     5.0
DATE          8      1    1977
TIMF          800    TO   1800     LOCAL DAYLIGHT TIME
SOLAR NOON    1314

DILUTION DETERMINED FROM THF FOLLOWING
INVERSION HEIGHTS      INITIAL    425.     FINAL      1900.
TIMING                 START      800.     STOP       1500.

INITIAL PROPYLENE FRACTION     .250     NO2/NOX    .250
INITIAL ALDEHYDF FRACTION      .050

TRANSPORTED CONCENTRATIONS
ALOFT                  OZONE     .100     HYDROCARBON   .000    NOX   .000 PPM

CONTINUOUS EMISSIONS (EXPRESSED AS THE FRACTION OF
INITIAL NON-BACKGROUND CONCENTRATION EMITTED PER HOUR)
HOUR         1      2      3
FRACTION  .360   .160   .070
```

Figure E-2 (continued)

```
                                        CITY-SPECIFIC EXAMPLE

THE ERROR TOLERANCE IS   1.000-02

THE RATE CONSTANTS USED WERE

    2.058-01   4.400+06   2.500+01   4.500-02   1.300+04   1.300+04   5.600+03   2.200+01   5.000-02   2.000-05
    1.000-03   1.196-02   8.000+03   3.000+03   1.200+03   8.400+03   4.579-04   2.882-04   1.705-02   8.700+10
    1.000+10   8.400+01   2.400+00   2.500+04   1.000+03   1.200+04   1.000+03   1.000+03   1.000+03   1.000+05
    8.000-03   8.000-03   1.800+03   1.800+03   1.800+03   1.800+03   1.800+03   1.800+03   1.800+03   7.500+04
    1.000+05   8.000+03   4.000+03   1.500+05   3.000+05   1.000+05   8.000+04   8.000+04   1.615-03   4.926-04
    1.500+04   4.200-06   2.031-04   1.500+04   6.000-05   2.500-03   4.500+04   6.000-05   1.900-03   4.500+04
    1.000+03   1.000+03   8.000+02   8.000+02   8.000+02   1.000+02   1.000+02   1.000+02   4.000+03   4.000+03
    4.000+03   4.000+03   4.000+03   4.000+03   4.000+03   4.000+03

THE PHOTOLYSIS REACTIONS ARE

          1         12         19         18         50         49         17         53

THE PHOTOLYTIC RATE CONSTANTS ARE

       2.058-01   1.196-02   1.705-02   2.882-04   4.926-04   1.615-03   4.579-04   2.031-04
```

Figure E-2 (continued)

```
                            TIME      HC       PROPYLENE     ALDEHYDE     NOX        NO2        OZONE
                            (LDT )    TOTAL    FRACTION      FRACTION     TOTAL      FRACTION   (INSTANT)

                            800.      1.00000   .25000        .05000      .21000     .25000     .00000

  TIME        NO2          NO          O           O3          NO3         N205        HONO        OH          HO2         HOOH
INTERVAL      O1D          PROP        ADD         X           MEO2        MEO         C202        C20         C302        C30
              HCHO         ALD2        C203        BUT         SC02        C402        C40         SCO         ALD4        ALD3
              C303         C403
 8.000+02     5.250-02     1.575-01    0.000       0.000       0.000       0.000       0.000       0.000       0.000       0.000
 1.000-10     0.000        8.333-02    0.000       0.000       0.000       0.000       0.000       0.000       0.000       0.000
              2.000-02     1.500-02    0.000       1.875-01    0.080       0.000       0.000       0.000       0.000       0.000
              0.000        0.000

NET RATES    -1.083-02     1.171-02    1.080-02    3.566-04    0.000       0.000       3.307-07    0.000       2.275-05    0.000
              0.000        3.510-04    0.000       0.000       3.046-06    0.000       0.000       0.000       0.000       0.000
              4.210-05     6.007-05    0.000       7.898-04    0.000       0.000       0.000       0.000       0.000       0.000
              0.000        0.000


THE REACTION RATES ARE
      1.08-02      0.00        0.00        0.00        0.00        0.00        0.00        0.00        0.00        1.65-07
      0.00         0.00        0.00        0.00        0.00        0.00        0.00        0.00        0.00        0.00
      0.00         0.00        0.00        0.00        0.00        0.00        0.00        0.00        0.00        0.00
      0.00         0.00        0.00        0.00        0.00        0.00        0.00        0.00        0.00        0.00
      0.00         0.00        0.00        0.00        0.00        0.00        0.00        0.00        0.00        0.00
      0.00         6.30-08     3.05-06     0.00        0.00        0.00        0.00        0.00        3.23-05     9.85-06
      0.00         0.00        0.00        0.00        0.00        0.00        0.00        0.00        0.00        0.00
      0.00         0.00        0.00        0.00        0.00        0.00
THE PHOTOLYTIC RATE CONSTANTS ARE

        2.058-01     1.196-02     1.705-02     2.882-04     4.926-04     1.615-03     4.579-04     2.031-04
```

Figure E-2 (Continued)

```
                                     TIME        HC       PROPYLENE      ALDEHYDE       NOX          NO2          OZONE
                                     (LDT )      TOTAL    FRACTION       FRACTION       TOTAL        FRACTION     (INSTANT)

                                     900.        1.06317   .23397        .07178         .22767       .39099       .00831

 TIME          NO2          NO           O            O3           NO3          N2O5         HONO         OH           HO2          HOOH
 INTERVAL      O1D          PROP         ADD          X            MEO2         MEO          C2O2         C2O          C3O2         C3O
               HCHO         ALD2         C2O3         BUT          SCO2         C4O2         C4O          SCO          ALD4         ALD3
               C3O3         C4O3
  9.000+02     8.902-02     1.387-01     6.729-09     8.313-03     1.706-08     3.626-07     1.262-03     1.135-07     2.959-06     1.377-0
  1.244+01     7.826-17     8.292-02     1.676-06     2.366-09     2.157-07     6.940-10     5.918-08     1.811-10     7.539-08     1.793-1
               2.746-02     2.443-02     3.796-07     2.036-01     1.635-07     1.635-07     1.853-10     1.042-10     8.421-04     4.756-0
               1.834-08     3.308-08

 NET RATES     7.485-06    -2.133-04     2.629-05     8.706-04     2.017-06     5.082-07     1.771-05    -1.116-05     1.167-05     6.747-01
               4.149-07    -2.579-04     2.764-06    -4.116-06     4.604-07    -1.684-06     3.078-07    -4.411-07     3.456-07    -5.519-0
               1.276-04     1.780-04     1.605-06    -1.700-04     7.815-07     7.815-07    -8.684-07    -8.684-07     1.883-05     1.259-0
               2.311-07     3.372-07

 THE REACTION RATES ARE
       2.94-02      2.96-02      2.88-02      3.33-05      7.79-06      3.08-05      8.51-06      7.98-06      1.81-08      2.47-0
       1.59-09      2.55-05      8.08-05      4.72-05      4.92-04      7.36-08      1.18-09      8.01-06      1.95-04      6.81-0
       7.83-07      7.93-08      5.90-08      2.35-04      2.32-04      3.37-08      3.62-10      9.92-11      1.26-10      2.37-0
       5.51-06      5.51-06      4.16-05      4.16-05      4.08-05      4.08-05      1.88-05      1.48-05      5.38-05      1.39-0
       1.04-05      1.43-06      7.24-07      2.78-05      3.13-05      1.79-05      1.45-05      5.55-05      8.26-05      2.70-0
       4.68-05      1.03-07      1.15-05      4.16-05      2.85-08      1.19-06      2.43-06      5.05-08      1.60-06      4.30-0
       2.74-10      2.74-10      3.67-06      2.03-06      4.21-05      2.94-07      1.63-07      3.38-06      1.94-09      8.92-1
       1.94-09      7.01-10      2.55-09      3.92-10      2.17-10      4.49-09

 THE PHOTOLYTIC RATE CONSTANTS ARE

         3.307-01     2.021-02     2.395-02     9.631-04     9.841-04     3.008-03     8.545-04     4.692-04
```

Figure E-2 (continued)

```
                          TIME      HC       PROPYLENE    ALDEHYDE     NOX         NO2        OZONE
                         (LDT )    TOTAL     FRACTION     FRACTION    TOTAL      FRACTION   (INSTANT)

                          1000.    .88886     .20057       .11409     .19618      .65288      .03020


 TIME         NO2         NO          O           O3          NO3         N205        HONO        OH          HO2         HOOH
INTERVAL      O1D         PROP        ADD         X           MEO2        MEO         C202        C20         C302        C30
              HCHO        ALD2        C203        BUT         SCO2        C402        C40         SCO         ALD4        ALD3
              C303        C403
 1.000+03    1.281-01    6.810-02    1.201-08    3.020-02    1.942-07    6.288-06    1.610-03    1.941-07    9.728-06    1.807-05
 1.244+01    5.825-16    5.943-02    4.229-06    2.882-09    9.601-07    1.472-09    2.557-07    3.735-10    3.079-07    3.497-10
             3.366-02    3.385-02    1.676-06    1.776-01    5.057-07    5.057-07    2.757-10    1.551-10    1.908-03    1.368-03
             1.773-07    2.474-07

NET RATES    3.960-04   -1.111-03    6.026-06    6.127-04    1.096-06    6.640-07   -6.037-06   -3.3 3-07    4.954-07    7.099-07
            -4.307-08   -4.445-04   -5.000-08    1.839-07    7.714-08   -7.688-08    2.239-08   -2.668-08    2.384-08   -2.742-08
             6.664-05    1.188-04    4.777-08   -5.474-09    5.137-08    5.137-08   -3.620-08   -3.620-08    1.414-05    1.465-05
             1.071-08    1.102-08
                 ,

THE REACTION RATES ARE
     5.20-02     5.29-02     5.14-02     1.74-04     2.00-05     1.72-04     1.39-04     1.38-04     3.14-07     1.74-07
     2.59-09     4.03-05     1.99-04     3.97-05     7.95-04     7.95-07     2.06-08     5.65-05     8.26-04     5.07-05
     5.82-06     4.92-07     7.05-07     2.88-04     2.88-04     2.15-07     4.06-09     1.08-09     1.30-09     2.88-04
     1.44-05     1.44-05     6.71-05     6.21-05     6.20-05     6.20-05     3.77-05     3.13-05     1.18-04     2.07-05
     1.55-05     2.80-06     1.49-06     4.14-05     4.65-05     3.50-05     2.99-05     1.18-04     1.34-04     4.72-05
     9.80-05     1.42-07     2.50-05     9.86-05     8.21-08     3.42-06     1.19-05     1.14-07     3.63-06     1.67-05
     7.19-09     2.14-09     1.35-05     9.66-06     9.13-05     3.17-06     2.27-06     2.15-05     1.97-08     1.20-08
     1.97-08     9.95-09     3.74-08     9.63-09     6.90-09     6.52-08

THE PHOTOLYTIC RATE CONSTANTS ARE

       4.061-01     2.503-02     2.736-02     1.870-03     1.402-03     3.973-03     1.140-03     7.382-04
```

Figure E-2 (continued)

```
                                   TIME       HC        PROPYLENE     ALDEHYDE       NOX          NO2         OZONE
                                  (LDT )     TOTAL       FRACTION     FRACTION      TOTAL       FRACTION    (INSTANT)

                                  1100.      .67768       .15350       .16177       .15052       .83232       .08668


   TIME          NO2          NO           O            O3           NO3          N205         HONO         OH           HO2          HOOH
 INTERVAL        OID          PROP         ADD          X            MEO2         MEO          C202         C20          C302         C30
                 HCHO         ALD2         C203         BUT          SCO2         C402         C40          SCO          ALD4         ALD3
                 C303         C403
   1.100+03      1.253-01     2.524-02     1.362-08     8.668-02     1.495-06     4.634-05     9.694-04     2.617-07     2.769-05     1.642-04
   1.423+01      2.444-15     3.467-02     8.876-06     2.274-09     3.104-06     1.793-09     8.577-07     4.725-10     9.657-07     4.133-10
                 3.449-02     3.757-02     5.172-06     1.434-01     1.460-06     1.460-06     2.998-10     1.686-10     2.429-03     2.009-03
                 7.093-07     8.595-07

 NET RATES      -1.209-03     3.239-04    -6.445-05     1.933-03     2.003-05    -8.027-06    -1.115-05    -1.192-05     1.174-05     5.634-06
                 9.654-07    -3.986-04     8.446-07    -1.460-06     7.884-07    -2.403-06     4.402-07    -7.190-07     4.601-07    -7.576-07
                -5.702-05    -1.135-05     1.695-06    -6.464-04     1.049-06     1.049-06    -1.113-06    -1.113-06     2.983-06     5.374-06
                 3.649-07     3.882-07

 THE REACTION RATES ARE
       5.71-02      5.99-02      5.47-02      4.89-04      2.22-05      4.74-04      1.01-03      1.02-03      2.32-06      6.32-08
       9.40-10      2.76-05      2.62-04      1.98-05      8.39-04      6.44-06      2.23-07      2.38-04      2.58-03      2.13-04
       2.44-05      1.91-06      5.76-06      2.27-04      2.24-04      9.45-07      2.76-08      7.61-09      8.57-09      2.27-04
       2.40-05      2.40-05      6.75-05      6.75-05      6.63-05      6.63-05      4.39-05      3.90-05      1.41-04      2.25-05
       1.69-05      3.31-06      1.89-06      4.50-05      5.06-05      4.13-05      3.78-05      1.43-04      1.63-04      5.92-05
       1.35-04      1.58-07      3.59-05      1.47-04      1.21-07      5.02-06      2.37-05      1.46-07      4.62-06      2.86-05
       1.30-08      1.30-08      1.74-05      1.43-05      1.04-04      1.08-05      8.89-06      6.48-05      1.62-07      1.07-07
       1.62-07      9.50-08      3.44-07      9.52-08      7.86-08      5.73-07

 THE PHOTOLYTIC RATE CONSTANTS ARE

         4.558-01     2.850-02     2.976-02     2.747-03     1.718-03     4.708-03     1.356-03     9.551-04
```

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Figure E-2 (continued)

```
                              TIME      HC        PROPYLENE    ALDEHYDE     NOX       NO2         OZONE
                             (LOT )    TOTAL      FRACTION     FRACTION    TOTAL     FRACTION    (INSTANT)

                             1200.     .48401      .10062       .19604     .10230     .88829      .14797

  TIME         NO2          NO           O           O3           NO3         N2O5        HONO        OH          HO2         HO2H
 INTERVAL      O1D          PROP         ADD         X            MEO2        MEO         C2O2        C2O         C3O2        C3O
               HCHO         ALD2         C2O3        RUT          SCO2        C4O2        C4O         SCO         ALD4        ALD3
               C3O3         C4O3
  1.200+03     9.087-02     1.193-02     1.114-08    1.480-01     4.035-06    9.335-05    4.711-09    3.063-07    4.739-05    7.892-09
  1.423+01     5.169-15     1.623-02     1.068-05    1.242-09     5.981-06    1.533-09    1.766-06    4.329-10    1.929-06    3.676-10
               2.818-02     3.335-02     9.358-06    1.088-01     2.887-06    2.887-06    2.691-10    1.485-10    2.323-03    2.028-03
               1.515-06     1.735-06

NET RATES     -5.172-09    -1.862-09    -1.050-05    7.521-04     6.283-06   -5.518-06   -5.460-06    1.178-06   -1.022-06    1.488-08
              -9.711-08    -2.206-04    -7.023-07    7.321-07     6.454-08    3.969-08    1.911-08   -1.079-08    1.757-08   -5.852-09
              -1.377-09    -1.160-04     4.100-08   -5.080-04     2.597-08    2.547-08   -2.694-09   -2.692-09   -5.234-06   -3.606-06
               4.190-08     4.201-08

THE REACTION RATES ARE
      4.39-02      4.90-02      4.23-02      6.05-04      1.32-05      5.99-04      2.05-03      2.05-03      4.67-06      2.08-08
      2.22-10      1.43-05      2.23-04      1.05-05      6.50-04      1.89-05      1.17-06      5.01-04      4.64-03      4.49-04
      5.16-05      3.81-06      1.68-05      1.24-04      1.22-04      1.37-06      6.37-08      1.89-08      2.06-08      1.24-04
      1.92-05      1.92-05      6.00-05      6.00-05      5.94-05      5.94-05      3.97-05      3.63-05      1.23-04      1.98-05
      1.49-05      2.94-06      1.73-06      3.96-05      4.46-05      3.68-05      3.46-05      1.23-04      1.49-04      5.39-05
      1.29-04      1.40-07      3.66-05      1.53-04      1.22-07      5.07-06      2.79-05      1.39-07      4.41-06      3.20-05
      3.08-08      3.08-08      1.59-05      1.38-05      8.56-05      1.58-05      1.38-05      8.50-05      5.47-07      3.66-07
      5.47-07      3.35-07      1.13-06      3.29-07      2.87-07      1.77-06

THE PHOTOLYTIC RATE CONSTANTS ARE

        4.833-01     3.090-02     3.136-02     3.385-03     1.914-03     5.122-03     1.984-03     1.098-03
```

Figure E-2 (continued)

```
                          TIME      HC      PROPYLENE    ALDEHYDE     NOX       NO2       OZONE
                          (LDT )    TOTAL   FRACTION     FRACTION     TOTAL     FRACTION  (INSTANT)

                          1300.     .34851   .05925       .20207      .06590    .90567    .18170


 TIME         NO2         NO          O          O3          NO3         N205        HONO        OH          HO2         HOOH
INTERVAL      O1D         PROP        ADD        X           HEO2        HEO         C202        C20         C302        C30
              HCHO        ALD2        C203       BUT         SCO2        C402        C40         SCO         ALD4        ALD3
              C303        C403
 1.300+03     5.968-02    6.216-03    8.161-09   1.817-01    5.981-06    9.067-05    2.504-04    3.394-07    5.647-05    1.802-03
 1.000+01     6.883-15    6.883-03    9.048-06   5.841-10    8.108-06    1.135-09    2.666-06    3.556-10    2.893-06    3.001-10
              1.972-02    2.535-02    1.244-05   8.197-02    4.378-06    4.378-06    2.180-10    1.226-10    1.925-03    1.703-03
              2.327-06    2.630-06

NET RATES    -4.561-04   -5.227-05   -2.134-07   3.562-04    3.614-07   -5.392-07   -2.353-06   -8.777-08    1.559-07    1.759-05
              2.112-09   -1.029-04   -4.569-08   1.160-09    3.687-08   -2.378-08    2.200-08   -1.107-08    2.374-08   -1.207-08
             -1.351-04   -1.398-04    6.336-08  -3.924-04    4.584-08    4.584-08   -1.997-08   -1.997-08   -7.345-06   -6.442-06
              1.911-08    2.146-08


THE REACTION RATES ARE
      2.95-02     3.59-02     2.82-02     4.88-04     6.33-06     4.83-04     2.00-03     1.99-03     4.53-06     7.42-09
      6.27-11     7.80-06     1.62-04     6.33-06     4.21-04     2.68-05     2.77-06     6.68-04     5.82-03     5.99-04
      6.88-05     5.18-06     2.46-05     5.84-05     5.62-05     9.82-07     7.34-08     2.41-08     2.62-08     5.84-05
      1.00-05     1.00-05     5.01-05     5.01-05     4.90-05     4.90-05     3.24-05     2.98-05     9.07-05     1.63-05
      1.23-05     2.40-06     1.42-06     3.27-05     3.68-05     3.00-05     2.84-05     9.08-05     1.04-04     3.94-05
      1.00-04     1.06-07     2.94-05     1.29-04     1.02-07     4.26-06     2.60-05     1.16-07     3.66-06     2.94-05
      3.96-08     3.96-08     1.31-05     1.16-05     6.19-05     1.57-05     1.39-05     7.43-05     9.89-07     6.53-07
      9.89-07     6.02-07     1.83-06     5.94-07     5.26-07     2.81-06

THE PHOTOLYTIC RATE CONSTANTS ARE

        4.942-01     3.117-02     3.202-02     3.674-03     1.997-03     5.297-03     1.538-03     1.159-03
```

Figure E-2 (continued)

```
                           TIME        HC       PROPYLENE    ALDEHYDE     NOX         NO2        OZONE
                           (LDT )      TOTAL    FRACTION     FRACTION     TOTAL       FRACTION   (INSTANT)

                           1400.       .25300    .03202       .18766      .04052      .91155     .19317

  TIME         NO2          NO           O           O3          NO3         N205        HONO        OH          HO2         HOOH
 INTERVAL      O1D          PROP         ADD         X           MEO2        MEO         C202        C20         C302        C30
               HCHO         ALD2         C203        BUT         SC02        C402        C40         SCO         ALD4        ALD3
               C303         C403
  1.400+03     3.693-02     3.583-03     5.652-09    1.932-01    6.823-06    6.406-05    1.500-04    3.695-07    5.779-05    2.777-03
  2.000+01     7.120-15     2.701-03     6.658-06    2.497-10    9.483-06    7.657-10    3.601-06    2.775-10    3.928-06    2.355-10
               1.258-02     1.745-02     1.483-05    6.122-02    6.085-06    6.065-06    1.746-10    9.820-11    1.491-03    1.311-03
               3.197-06     3.634-06

 NET RATES    -2.932-04    -4.471-05    -2.739-06    4.069-05    1.396-06   -1.680-06   -1.191-04    6.431-07   -4.109-07    1.394-05
              -1.205-06    -4.292-05    -1.945-07    1.492-07    1.083-08   -2.642-08    5.032-08   -5.599-08    5.567-08   -6.431-08
              -9.875-05    -1.177-04     8.939-08   -2.997-04    1.276-07    1.276-07   -1.162-07   -1.162-07   -6.832-06   -6.287-06
               7.393-08     9.129-08

 THE REACTION RATES ARE
       1.81-02       2.49-02       1.73-02       3.21-04       2.71-06       3.18-04       1.41-03       1.41-03       3.20-06       2.65-09
       2.25-11       4.63-06       1.09-04       3.97-06       2.49-04       2.81-05       4.22-06       6.89-04       6.14-03       6.19-04
       7.12-05       5.99-06       2.68-05       2.49-05       2.39-05       5.32-07       6.31-08       2.40-08       2.62-08       2.50-05
       4.17-06       4.17-06       4.07-05       4.07-05       3.91-05       3.91-05       2.53-05       2.32-05       6.12-05       1.31-05
       9.82-06       1.88-06       1.11-06       2.62-05       2.95-05       2.35-05       2.22-05       6.13-05       6.59-05       2.48-05
       6.97-05       7.33-08       1.98-05       9.67-05       7.87-08       3.28-06       2.18-05       8.94-08       2.83-06       2.48-05
       4.04-08       4.04-08       1.04-05       9.17-06       4.25-05       1.34-05       1.18-05       5.48-05       1.40-06       9.08-07
       1.40-06       8.33-07       2.19-06       8.40-07       7.39-07       3.43-06

 THE PHOTOLYTIC RATE CONSTANTS ARE

         4.904-01      3.090-02      3.179-02      3.569-03      1.967-03      5.235-03      1.519-03      1.137-03
```

Figure E-2 (continued)

```
                                   TIME      HC        PROPYLENE     ALDEHYDE      NOX          NO2         OZONE
                                   (LDT )    TOTAL     FRACTION      FRACTION      TOTAL        FRACTION    (INSTANT)

                                   1500.     .18558    .01693        .16519        .02425       .91387      .19051


  TIME         NO2         NO          O           O3          NO3         N2O5        HONO        OH          HO2         HOOH
INTERVAL       O1D         PROP        ADD         X           MEO2        MEO         C2O2        C2O         C3O2        C3O
               HCHO        ALD2        C2O3        BUT         SCO2        C4O2        C4O         SCO         ALD4        ALD3
               C3O3        C4O3
  1.500+03     2.217-02    2.089-03    3.820-09    1.905-01    6.932-06    3.903-05    9.482-05    3.841-07    5.377-05    3.414-03
  9.281+00     6.069-15    1.047-03    4.509-06    1.007-10    1.086-05    4.735-10    4.523-06    2.027-10    4.990-06    1.739-10
               7.781-03    1.144-02    1.643-05    4.561-02    7.909-06    7.909-06    1.323-10    7.444-11    1.116-03    9.649-04
               4.059-06    4.695-06

NET RATES     -1.942-04   -1.929-05   -2.183-10   -1.141-04   -2.539-09   -3.491-07   -7.317-07   -1.705-11   -1.027-07    7.241-06
               2.728-12   -1.698-05   -2.636-08    4.145-11    1.584-09   -1.000-11    1.364-08   -2.501-12    1.608-08   -7.728-12
              -6.350-05   -8.321-05    1.586-08   -2.257-04    2.933-08    7.933-08   -1.329-12   -8.740-13   -5.612-06   -5.196-06
               1.204-08    1.561-08

THE REACTION RATES ARE
      1.04-02     1.88-02     9.95-03     1.90-04     1.10-06     1.88-04     8.60-04     8.59-04     1.95-06     9.26-10
      8.99-12     2.80-06     6.81-05     2.41-06     1.35-04     2.43-05     4.87-06     5.89-04     5.84-03     5.78-04
      6.07-05     6.15-06     2.46-05     1.01-05     9.42-06     2.44-07     4.54-08     2.04-08     2.25-08     1.01-05
      1.60-06     1.60-06     3.15-05     3.15-05     2.97-05     2.97-05     1.88-05     1.70-05     3.78-05     9.92-06
      7.44-06     1.39-06     8.11-07     1.98-05     2.23-05     1.74-05     1.62-05     3.79-05     3.84-05     1.42-05
      4.48-05     4.80-08     1.18-05     6.59-05     5.79-08     2.41-06     1.67-05     6.70-08     2.12-06     1.93-05
      3.57-08     3.57-08     7.85-06     6.78-06     2.75-05     1.04-05     9.00-06     3.64-05     1.70-06     1.07-06
      1.70-06     9.73-07     2.16-06     1.01-06     8.73-07     3.53-06

THE PHOTOLYTIC RATE CONSTANTS ARE

        4.712-01     2.956-02     3.064-02     3.090-03     1.826-03     4.933-03     1.427-03     1.033-03
```

Figure E-2 (continued)

```
                         TIME       HC       PROPYLENE    ALDEHYDE     NOX        NO2       OZONE
                         (LDT )     TOTAL    FRACTION     FRACTION     TOTAL      FRACTION  (INSTANT)

                         1600.      .16996   .00877       .14308       .01772     .92390    .20001

 TIME        NO2         NO         O          O3          NO3         N2O5        HONO        OH          HO2         HOOH
 INTERVAL    O1D         PROP       ADD        X           MEO2        MEO         C2O2        C2O         C3O2        C3O
             HCHO        ALD2       C2O3       RUT         SCO2        C4O2        C4O         SCO         ALD4        ALD3
             C3O3        C4O3
 1.600+03    1.637-02    1.349-03   3.005-09   2.000-01    8.306-06    3.455-05    6.784-05    3.372-07    4.851-05    4.431-03
 7.000+01    4.752-15    4.970-04   2.888-06   4.209-11    9.909-06    3.011-10    5.300-06    1.534-10    5.913-06    1.331-10
             5.910-03    9.204-03   1.628-05   4.212-02    9.732-06    9.732-06    1.051-10    5.914-11    1.016-03    8.542-04
             4.454-06    5.297-06

 NET RATES   -8.087-05   -8.709-06  -2.196-07  1.191-04    2.543-07    -2.339-07   -4.593-07   1.182-11    -1.250-07   1.422-05
             -9.746-08   -5.780-06  -2.278-08  3.907-09    -1.151-08   -6.776-10   1.069-08    -2.086-09   1.271-08    -1.725-09
             -2.626-05   -3.123-05  -2.240-08  -5.113-05   2.489-08    2.432-08    -1.679-09   -1.678-09   -1.640-06   -1.843-06
             -7.923-10   1.750-09


 THE REACTION RATES ARE
     7.09-03     1.32-02     6.74-03     1.47-04     6.40-07     1.46-04     7.62-04     7.60-04     1.73-06     4.42-10
     4.60-12     1.82-06     4.42-05     1.36-06     7.85-05     1.98-05     5.56-06     4.61-04     5.72-03     4.13-04
     4.75-05     5.67-06     2.33-05     4.19-06     3.90-06     1.00-07     2.86-08     1.53-08     1.71-08     4.21-06
     7.95-07     7.95-07     2.56-05     2.56-05     2.36-05     2.36-05     1.44-05     1.29-05     2.41-05     7.88-06
     5.91-06     1.06-06     6.13-07     1.58-05     1.77-05     1.33-05     1.23-05     2.41-05     2.58-05     9.26-06
     2.99-05     3.87-08     7.82-06     4.66-05     5.13-08     2.14-06     1.30-05     6.10-08     1.93-06     1.54-05
     2.81-08     2.81-08     5.72-06     4.81-06     1.76-05     8.67-06     7.29-06     2.67-05     1.89-06     1.15-06
     1.89-06     1.03-06     1.92-06     1.03-06     8.64-07     3.16-06

 THE PHOTOLYTIC RATE CONSTANTS ARE

       4.329-01     2.690-02     2.860-02     2.304-03     1.567-03     4.358-03     1.254-03     8.496-04
```

Figure E-2 (continued)

```
                         TIME      HC        PROPYLENE    ALDEHYDE     NOX        NO2         OZONE
                        (LDT )    TOTAL      FRACTION     FRACTION     TOTAL      FRACTION   (INSTANT)

                         1700.    .15888      .00490       .12599      .01338      .93572      .20517

  TIME          NO2         NO          O           O3          NO3         N2O5        HONO        OH          HO2         HOOH
 INTERVAL       O1D         PROP        ADD         X           MEO2        MEO         C2O2        C2O         C3O2        C3O
                HCHO        ALD2        C2O3        BUT         SCO2        C4O2        C4O         SCO         ALD4        ALD3
                C3O3        C4O3
 1.700+03     1.252-02    8.600-04    2.304-09    2.052-01    1.016-05    3.234-05    4.336-05    2.457-07    3.912-05    5.090-03
 2.000+01     2.919-15    2.598-04    1.703-06    1.609-11    8.531-06    1.650-10    5.456-06    1.005-10    6.115-06    8.750-11
              4.616-03    7.701-03    1.380-05    3.953-02    1.029-05    1.029-05    7.059-11    3.971-11    9.235-04    7.529-04
              3.989-06    4.894-06

 NET RATES   -4.895-05   -6.268-06   -1.912-06    5.914-05    1.503-06   -1.083-06   -3.510-07    6.725-08   -2.038-07    7.770-06
              2.648-07   -2.448-06   -8.254-09   -5.200-09   -3.495-08    2.119-08   -1.256-08    1.696-08   -1.683-08    2.563-08
             -1.704-05   -1.899-05   -1.213-07   -3.496-05   -8.690-08   -8.690-08    7.162-08    7.162-08   -1.431-06   -1.500-06
             -3.935-08   -5.090-08

 THE REACTION RATES ARE
     4.64-03     1.01-02     4.41-03     1.16-04     3.75-07     1.14-04     7.12-04     7.11-04     1.62-06     2.15-10
     1.88-12     9.85-07     2.46-05     6.34-07     4.04-05     1.29-05     5.08-06     2.83-04     5.24-03     2.54-04
     2.92-05     4.23-06     1.93-05     1.60-06     1.46-06     3.48-08     1.45-08     9.29-09     1.04-08     1.61-06
     4.26-07     4.26-07     1.75-05     1.75-05     1.59-05     1.59-05     9.47-06     8.45-06     1.32-05     5.29-06
     3.97-06     7.00-07     4.02-07     1.06-05     1.19-05     8.75-06     8.04-06     1.32-05     1.62-05     5.51-06
     1.70-05     3.23-08     4.63-06     2.84-05     4.52-08     1.88-06     8.32-06     5.54-08     1.75-06     1.02-05
     1.75-08     1.75-08     3.37-06     2.74-06     9.49-06     6.13-06     4.99-06     1.73-05     1.61-06     9.57-07
     1.61-06     8.54-07     1.33-06     7.66-07     6.24-07     2.16-06

 THE PHOTOLYTIC RATE CONSTANTS ARE

       3.705-01    2.272-02    2.556-02    1.381-03    1.194-03    3.498-03    9.989-04    6.008-04
```

Figure E-2 (continued)

```
                       TIME      HC        PROPYLENE    ALDEHYDE    NOX       NO2        OZONE
                       (LDT )    TOTAL     FRACTION     FRACTION    TOTAL     FRACTION   (INSTANT)

                       1800.     .15209    .00314       .11533      .01080    .95242     .20742


 TIME        NO2         NO          O           O3          NO3         N2O5        HONO        OH          HO2         HOOH
INTERVAL     O1D         PROP        ADD         X           MEO2        MEO         C2O2        C2O         C3O2        C3O
             HCHO        ALD2        C2O3        BUT         SCO2        C4O2        C4O         SCO         ALD4        ALD3
             C3O3        C4O3
 1.800+03    1.029-02    5.138-04    1.634-09    2.074-01    1.375-05    3.609-05    2.588-05    1.316-07    2.726-05    5.401-03
 1.811+01    1.171-15    1.592-04    9.384-07    5.199-12    6.011-06    6.802-11    4.972-06    5.459-11    5.449-06    4.642-11
             3.812-03    6.865-03    9.057-06    3.790-02    8.800-06    8.800-06    3.580-11    2.014-11    8.434-04    6.756-04
             2.624-06    3.276-06

NET RATES   -1.313-05   -1.485-05   -3.331-05    3.742-05    6.359-06   -3.989-06   -2.184-07   -3.497-08   -6.748-07    2.700-06
             3.021-06   -1.052-06   -1.159-08    1.533-08   -5.781-08    1.240-07    7.348-09    1.773-08   -4.432-09    3.117-08
            -9.616-06   -8.633-06   -2.143-07   -1.795-05   -1.307-07   -1.307-07    9.313-08    9.313-08   -1.277-06   -1.088-06
            -6.293-08   -7.994-08

THE REACTION RATES ARE
      2.80-03     7.19-03     2.66-03     9.60-05     2.18-07     9.18-05     7.92-04     7.94-04     1.80-06     1.06-10
      6.70-13     4.21-07     1.08-05     2.03-07     1.68-05     6.24-06     3.54-06     1.17-04     4.26-03     1.02-04
      1.17-05     2.29-06     1.36-05     5.24-07     4.82-07     1.06-08     5.64-09     4.67-09     5.11-09     5.20-07
      2.64-07     2.64-07     8.98-06     8.98-06     8.14-06     8.14-06     5.04-06     4.60-06     5.56-06     2.68-06
      2.01-06     3.71-07     2.18-07     5.37-06     6.04-06     4.64-06     4.37-06     5.44-06     8.82-06     2.77-06
      7.52-06     2.88-08     2.22-06     1.35-05     4.05-08     1.69-06     4.00-06     5.06-08     1.60-06     4.99-06
      8.26-09     8.26-09     1.35-06     1.08-06     3.72-06     3.37-06     2.70-06     9.32-06     9.60-07     5.94-07
      9.60-07     5.42-07     6.55-07     3.57-07     2.86-07     9.87-07

THE PHOTOLYTIC RATE CONSTANTS ARE

        2.718-01    1.628-02    2.052-02    5.622-04    7.277-04    2.313-03    6.556-04    3.236-04

                 MAXIMUM OZONE NOT REACHED, THE LAST ONE HOUR AVERAGE WAS .20645 PPM.
```

Figure E-2 (continued)

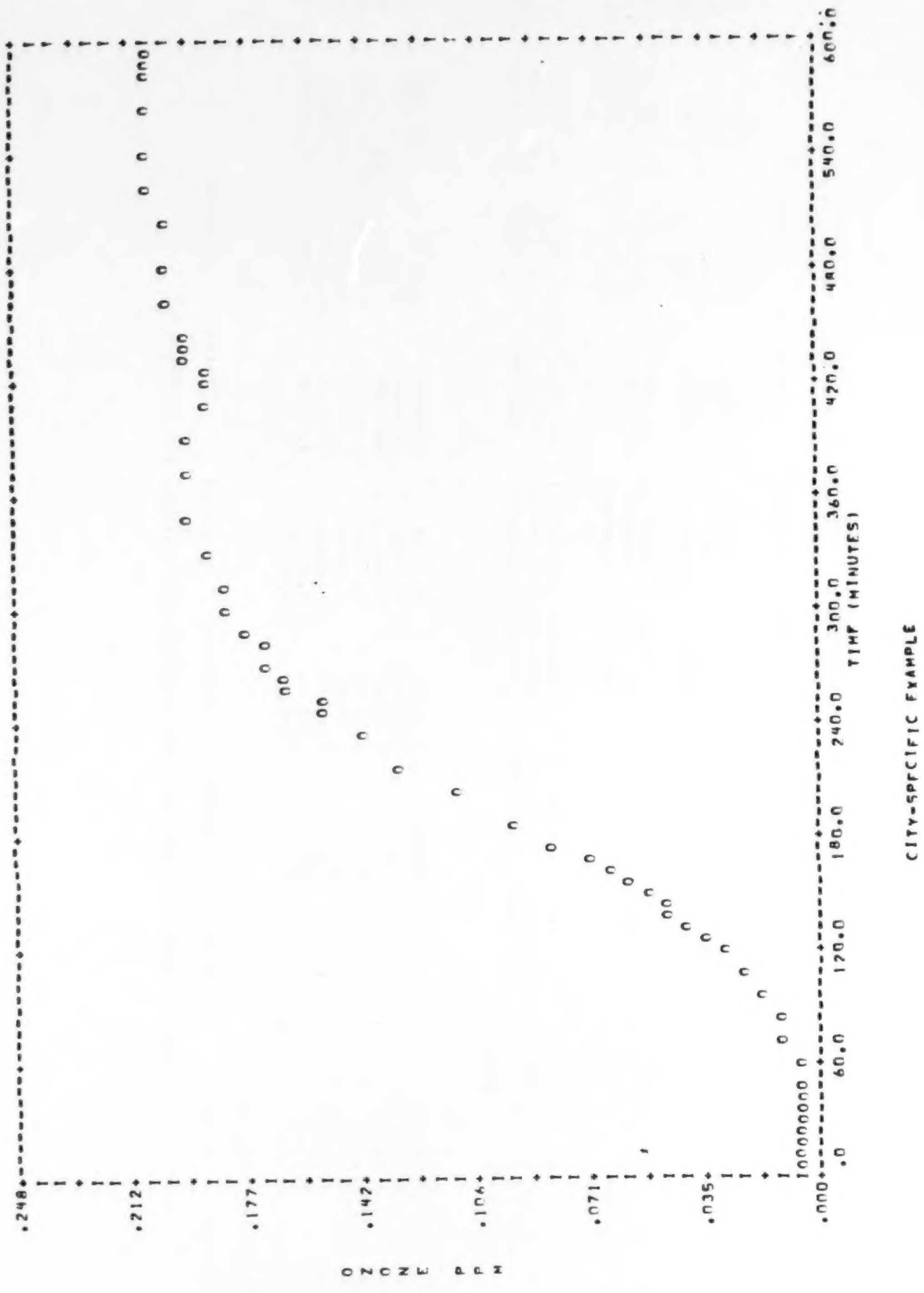

Figure E-2 (continued)

```
CITY-SPECIFIC EXAMPLE

PHOTOLYTIC RATE CONSTANTS CALCULATED FOR

          TEST RUN CITY

LATITUDE      39.000
LONGITUDE      77.000
TIME ZONE    5.0
DATE           8       1    1977 .
TIME          800    TO    1800       LOCAL DAYLIGHT TIME
SOLAR NOON   1314


DILUTION DETERMINED FROM THE FOLLOWING
INVERSION HEIGHTS        INITIAL    425.      FINAL       1900.
TIMING                   START      800.      STOP        1500.

INITIAL PROPYLENE FRACTION        .250       NO2/NOX    .250
INITIAL ALDEHYDE FRACTION         .050

TRANSPORTED CONCENTRATIONS
ALOFT
                         OZONE    .100      HYDROCARBON    .000     NOX    .000 PPM

CONTINUOUS EMISSIONS (EXPRESSED AS THE FRACTION OF
INITIAL NON-BACKGROUND CONCENTRATION EMITTED PER HOUR)
HOUR         1      2      3
FRACTION  .360   .160   .070
```

Figure E-2 (continued)

```
THE FOLLOWING SIMULATIONS WERE DONE.

          HC            NOX           RATIO          OZONE           TIME

DUE TO HIGH BACKGROUND CONDITIONS THE LOWEST OZONE PLOTTED WILL BE   .08 PPM.
       .18459         .14000         1.31847         .06861          567.
       .70000         .01628        42.98940         .11206          303.
       .50807         .10161         5.00000         .14965       NOT MAX
       .31094         .06219         5.00000         .12223       NOT MAX
       .16648         .03330         5.00000         .10000          434.
       .06667         .01333         5.00000         .08239          406.
       .60815         .14000         4.34391         .16210       NOT MAX
       .44830         .10320         4.34391         .14216       NOT MAX
       .27932         .06430         4.34391         .11820       NOT MAX
       .15305         .03523         4.34391         .09804          445.
       .06568         .01512         4.34391         .08258          409.
       .51629         .14000         3.68782         .14778       NOT MAX
       .38935         .10558         3.68782         .13250       NOT MAX
       .24728         .06705         3.68782         .11308       NOT MAX
       .13782         .03737         3.68782         .09554          457.
       .06451         .01749         3.68782         .08267          413.
       .42444         .14000         3.03172         .12917       NOT MAX
       .33191         .10948         3.03172         .12005       NOT MAX
       .21120         .06966         3.03172         .10588       NOT MAX
       .11869         .03915         3.03172         .09180          472.
       .06367         .02100         3.03172         .08271          421.
       .34586         .14000         2.47040         .10985       NOT MAX
       .28497         .11535         2.47040         .10627       NOT MAX
       .17239         .06978         2.47040         .09726       NOT MAX
```

Figure E-2 (continued)

```
.09351      .03785      2.47040     .08687      464.
.06113      .02474      2.47040     .08203      429.
.29330      .14000      2.09497     .09584   NOT MAX
.25629      .12234      2.09497     .09506   NOT MAX
.12815      .06117      2.09497     .08939   NOT MAX
.06407      .03058      2.09497     .08187      441.
.05767      .02753      2.09497     .08094      435.
.70000      .11290      6.20013     .16991      341.
.51031      .08231      6.20013     .14654   NOT MAX
.32054      .05170      6.20013     .12142      372.
.17221      .02777      6.20013     .09996      413.
.06877      .01109      6.20013     .08204      404.
.70000      .08580      8.15833     .16928      310.
.51075      .06260      8.15833     .14529      324.
.32675      .04005      8.15833     .12020      350.
.18314      .02245      8.15833     .09956      399.
.07503      .00920      8.15833     .08214      406.
.70000      .05946     11.77210     .16052      286.
.51722      .04394     11.77210     .13859      305.
.34196      .02905     11.77210     .11604      336.
.20019      .01701     11.77210     .09804      396.
.08686      .00738     11.77210     .08235      410.
.70000      .03477     19.03923     .14288      279.
.53249      .02797     19.03923     .12606      300.
.37020      .01944     19.03923     .10932      337.
.23143      .01216     19.03923     .09538      404.
.10976      .00576     19.03923     .08257      418.
.57266      .01332     42.98939     .10470      330.
.43433      .01010     42.98940     .09477      385.
```

Figure E-2 (continued)

```
.30244        .00704       42.98940        .08953        418.
.17770        .00413       42.98940        .08216        427.
.13566        .14000         .96901        .05911        521.
.70000        .00450      155.39421        .08386        418.
```

Figure E-2 (continued)

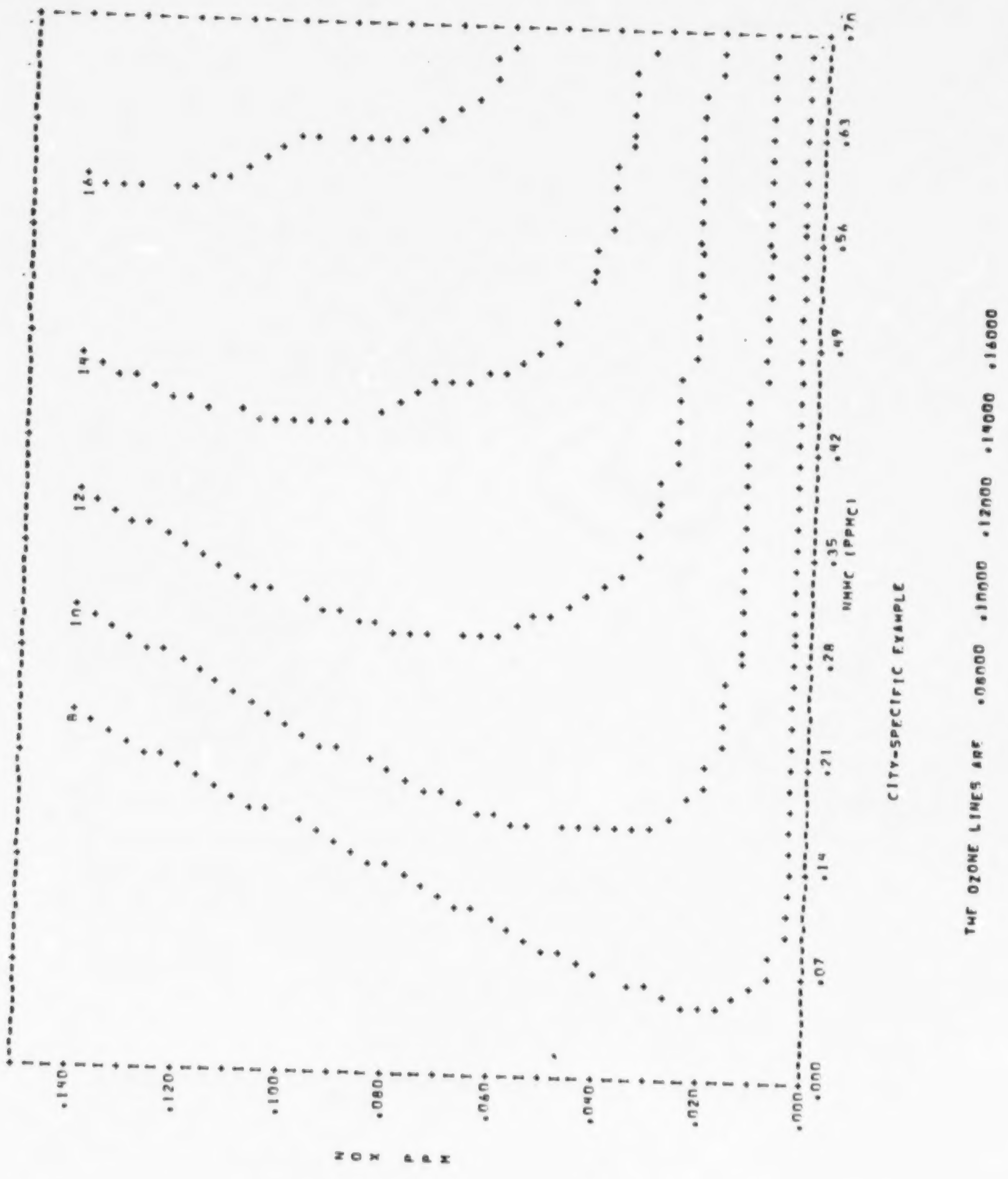

Figure E-2 (concluded)

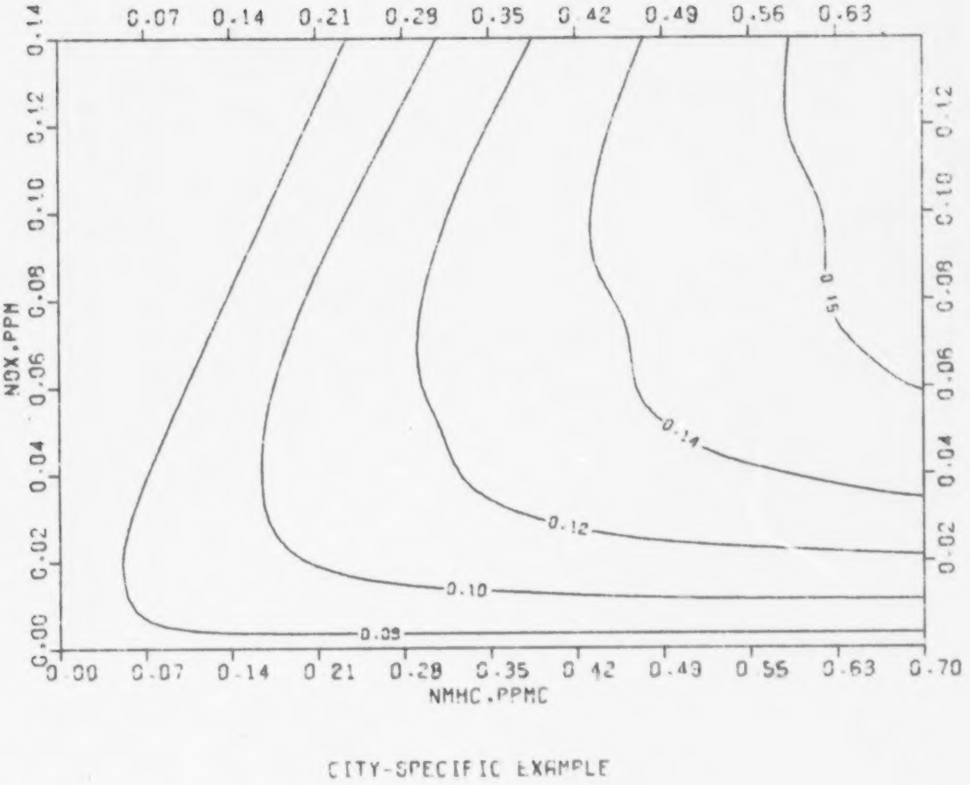

FIGURE E-3. CALCOMP Plot For City-Specific Diagram Example